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Donald L. Perry, C.C. Chuang, Gregory A. Jungclaus, and J. Scott Warner

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16. ABSTRACT

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Over 570 compounds were tentatively identified of which 33 are priority pollutants. Generally, industrial effluents contained few priority pollutants. Most of the components found in the effluents were specific for a particular industrial site and did not appear in reoccurring patterns. The data suggest that many possible environmentally important compounds would be overlooked if frequency of occurrence is the major criterion for determining environmentally significant compounds.

We recommend that future studies concentrate on basic compound analyses and that the biological activity of a compound(s) be established first before exhaustive screening programs are initiated for environmental pollutants. Mass spectral data bases containing all the organic compounds produced by industry should be developed.

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by

D. L. Perry, C. C. Chuang, G. A. Jungclaus,
and J. S. Warner

BATTELLE
Columbus Laboratories
505 King Avenue
Columbus, Ohio 43201

Contract No. 68-01-4350

Project Officers

Vincent J. DeCarlo
Office of Toxic Substances
U.S. Environmental Protection Agency
Washington, D.C. 20460

and

Ann Alford
Analytical Chemistry Branch
Environmental Research Laboratory
Athens, Georgia 30605

ENVIRONMENTAL RESEARCH LABORATORY
OFFICE OF RESEARCH AND DEVELOPMENT
U.S. ENVIRONMENTAL PROTECTION AGENCY
ATHENS, GEORGIA 30605

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FOREWARD

ABSTRACT

Samples of 63 effluent and 22 intake waters were collected from a wide range of chemical manufacturers in areas across the United States. The samples were analyzed for organic compounds in an effort to identify previously unknown and potentially hazardous organic pollutants. Each water sample was preconcentrated for analysis of organic compounds in four fractions: volatile organics by helium-gas stripping and semivolatile organics by extraction with methylene chloride resulting in separate neutral, acidic and basic fractions. All sample analyses involved a GC/MS/COMP system that used high-resolution glass capillary GC columns. Organic constituents were identified using the computerized Biemann mass spectral matching system together with some manual interpretation and quantified using GC-FID peak area determinations.

Over 570 compounds were tentatively identified of which 33 are priority pollutants. Generally, industrial effluents contained few priority pollutants. Most of the components found in the effluents were specific for a particular industrial site and did not appear in reoccurring patterns. The data suggest that many possible environmentally important compounds would be overlooked if frequency of occurrence is the major criterion for determining environmentally significant compounds.

We recommend that future studies concentrate on basic compound analyses and that the biological activity of a compound(s) be established first before exhaustive screening programs are initiated for environmental pollutants. Mass spectral data bases containing all the organic compounds produced by industry should be developed.

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INTRODUCTION

There has been an increasing concern in recent years that man and his environment are being exposed to unknown industrial pollutants which may represent significant hazards. One approach to assessing the potential hazards involves a detailed chemical characterization of waste effluents. The objective of this program was the identification and quantification of organic compounds present in representative industrial final aqueous effluents. The information obtained will help the U.S. Environmental Protection Agency in its efforts in determining the health and environmental effects of industrial effluents, determining transport and degradation mechanisms, developing and assessing monitoring and control technology, and assessing wastewater disposal permits.

Priority was given to major industrial activities that were most apt to have significant amounts of organic compounds in their final aqueous effluents. Four different fractions from each effluent sample were analyzed by gas chromatography (GC) and gas chromatography-mass spectrometry (GC-MS) procedures. The fractions were acidic and neutral volatiles, neutral semivolatiles, acidic semivolatiles, and basic semivolatiles.

The program was designed as a cursory survey of wastewater effluent samples. A computerized mass spectral search system was used as the basis for compound identifications. High-resolution glass capillary GC columns were used to obtain the best possible mass spectra from the GC/MS/COMP systems. Because of the large number of samples, this program provided for only limited manual mass spectral interpretation.

CONCLUSIONS AND RECOMMENDATIONS

The conclusions and recommendations concerning this project are divided into three categories: (1) those which deal with the analytical protocol used in this program; (2) those which deal with the analytical results obtained; and (3) those concerned with the design of future studies for detecting environmentally significant pollutants.

ANALYTICAL PROTOCOL

- Stringent quality assurance protocols, such as those established for this program, must be followed during the performance of each analysis. Particularly important are instrument calibration (GC/MS/COMP), process and field blanks, uniformity of capillary GC system performance and recovery of representative standard compounds from spiked samples.
- Capillary column GC/MS for volatile analysis was demonstrated in this program to be a sensitive and specific method suitable for routine work. The improved resolution of the capillary column (compared to packed columns) provides well resolved peaks which result in cleaner mass spectra and thus more certain identification of the various volatile compounds. However, capillary columns are not the answer for every analytical problem.
- Basic priority pollutants were not found in the industrial effluents using SE-30 glass capillary columns. Benzidine and 3,3'-dichlorobenzidine could only be detected reliably at levels of greater than 50 μg/l with our method. Consequently, if lower detection limits are necessary for benzidine analysis, more suitable methods should be used. One such method is the electrochemical detection of benzidines following HPLC separation.
- Mass spectral and relative retention time data bases containing most, if not all, of the organic compounds produced by industry should be developed. Present data bases contain mass spectra of less than 20% of the presently manufactured industrial compounds. Consequently, identification of "unknown" pollutants was difficult due to the incomplete data bases of the mass spectral matching systems. Manual

interpretation procedures are not feasible for a screening project of this scale.

- The majority of pollutants present at levels greater than 10 µg/l were tentatively identified. However, there is considerable uncertainty associated with some of the interpretations. In general the most common and most frequently studied compounds (i.e., hydrocarbons, halocarbons, fatty acids, and phenols) are identified with a high degree of certainty. Pollutants which have not been previously identified are of particular interest in this type of study but they are less likely to be included in data bases and less likely to be correctly identified.

- The Biemann computer mass spectral matching system does provide a useful "first guess" in the identification of an unknown compound, but it is unreliable in determining the degree of certainty of a particular compound identification. Thus, the computer generated GC/MS data alone are not sufficient evidence for the positive identification of "unknown" compounds. Retention time data and manual interpretation must be used.

- Many samples contained only a few components as determined by preliminary GC analysis, whereas others contained many compounds in high concentrations. Consequently, the GC screening procedure used (i.e., priority rating system) saved time and money by determining which samples contained a sufficient number of components above a specified concentration level (10 µg/l) to warrant subsequent GC/MS/COMP analysis. However, the relatively few contaminants present in those samples not analyzed by GC/MS may have been potentially toxic components that should be of concern.

ANALYTICAL RESULTS

- Caution should be used when interpreting the analytical data, especially the frequency of occurrence tables, because this was only a limited study.

- Generally, industrial effluents contain few priority pollutants. In the semivolatile fractions only 17 priority pollutants were identified and these occurred collectively 78 times--only 10% of the 816 occurrences of semivolatile compounds. This percentage of occurrence of priority pollutants is the upper limit since the unidentified compounds would not be priority pollutants.

- Priority pollutants are most prevalent in the purgeable fractions of industrial effluents. This was expected since most of these compounds are common industrial solvents. Twenty-two priority pollutants were identified and occurred collectively 359 times--51% of the 710 occurrences of purgeable compounds.

- Most of the components found in the effluents were specific for a particular industrial site and did not appear in reoccurring patterns. Specifically, 176 out of 261 neutral compounds, 56 out of 104 acidic compounds, 39 out of 49 basic compounds, and 85 out of 159 volatile compounds occurred only once. These data suggest that many possible environmentally important compounds (mutagenic, toxic, carcinogenic) would be overlooked if frequency of occurrence is the major criterion for determining environmentally significant compounds.

- Few polycyclic aromatic hydrocarbons (PAH's) were identified in industrial effluents. This fact supports the combustion airborne hypothesis that PAH's enter the surface waters primarily as a result of the combustion of fossil fuels.

- Many different types of heterocyclic compounds appeared in the basic fraction. Such compounds are very likely toxic or mutagenic and may prove to be environmentally significant.

FUTURE STUDIES

- We recommend that future studies concentrate on basic compounds using suitable methods of identification and that appropriate tests for compound activity (toxicity, mutagenicity, carcinogenicity) be conducted.

- We recommend that future studies concerning the environmental impact of various compounds first identify which compounds are biologically active (toxicity, mutagenicity, carcinogenicity) and then apply suitable methods for their detection in the environment. This could be accomplished by fractionating extracts using liquid chromatography and screening the fractions by bioassay techniques (e.g., Ames mutagenicity assay, mammalian cell toxicity assay). Active fractions would be subfractionated and studied in detail to identify the biologically active components.

- The current study was concerned only with volatile and semivolatile components. The many nonvolatile organic components that were undoubtedly present and which may be biologically active were ignored. We recommend that future studies include efforts to identify biologically active nonvolatile components. This could be accomplished most efficiently by combining liquid chromatographic fractionation and bioassay techniques with HPLC-MS and HPLC/IR studies.

SAMPLING

SITE SELECTION

The objective of sampling site selection was to develop a sampling design system which allowed the collection of representative, usable and statistically reliable data concerning the possible source of organic pollutants entering receiving waters. A preliminary list of 478 organic chemical manufacturing facilities was compiled and classified according to type of chemical industry. Sampling sites were chosen from this list using the following criteria:

(1) Type of industry
(2) Potential toxicity of anticipated pollutants
(3) Production capacity of company
(4) Willingness of company to permit sampling

In retrospect, the main factor for site selection was the willingness of the company to permit sampling. The other major criterion was the type of industry to be considered. These industries included all types of organic chemical manufacturers and even steel manufacturers because of their coal tar production. Table 1 summarizes the various types of chemicals produced by these companies.

Letters were sent to 250 corporations requesting permission to sample at some 450 sites. Each company was informed that data obtained from their water samples would not be identified with their respective company. In this way each company's identity will remain confidential. Approximately 10% of the corporations contacted refused to participate. Many corporations (94 out of 250) had sampling sites (100) which discharged into municipal treatment plants. These sites were not applicable for this project since only those effluents which were discharged directly into surface waters were of interest. Eighteen corporations requested that intake water be analyzed as well as effluent water. In this way, chemicals identified as being introduced *via* the intake water would not be erroneously attributed to the manufacturing operations.

SAMPLE COLLECTION AND PRESERVATION

Samples were collected from sites in Ohio, West Virginia, Pennsylvania, New Jersey, New York, Louisiana, Kentucky, Delaware, and Texas. In total, samples of 63 outfalls and 22 intakes (plant water supply) were collected.

TABLE 1. CHEMICALS PRODUCED BY COMPANIES SAMPLED

rubber processing chemicals
plastics and resins
dyes, color agents and pigments
aromatic hydrocarbons
surface-active agents
tar, tar prods, petroleum prods.
carbon black
lecithin and derivatives
aliphatic solvents
medicinals or phameceuticals
industrial organic chemicals
organic acids and salts
fatty acids & derivatives
organic sufrace coatings
flavor and fragrance chemicals
pesticides
epoxys
miscellaneous organic chemicals
surfactants
elastomers
catalysts and catalyst supports
polymers
organic intermediates
synthetic fibers
paints and varnishes
enzymes
pulp and paper chemicals
silanes, silicones
leather finishes
chelating agents
amines
printing inks
peroxides
chlorine compounds
edible fats, oils, etc.
synthetic rubbers

Samples were collected in such a way as to provide as representative a sample as possible from each sampling site. This required close coordination with facilities personnel to ensure that sampling was performed during a representative stage of the production cycle. In many cases effluents from the various operations of a particular plant were pooled and may have been subjected to purification treatment prior to discharge. These pooled samples averaged many of the periodic fluctuations in the composition of the effluents and permitted a grab sample to be taken which was reasonably representative of several hours of operation. For this reason and because grab sampling is by far the least costly method, grab samples were collected at all the sites. Other advantages of grab sampling are that contamination is minimized and the sample can be immediately capped and cooled to prevent loss of volatile compounds.

Grab samples for analysis of semivolatile compounds were collected in pre-washed one-half gallon glass bottles containing 5 grams of potassium bisulfate ($KHSO_4$) and 75 grams of sodium chloride. Two bottles of sample were collected at each intake (or process water source) and process water outfall. Each bottle was filled approximately half full with sample water. Next, 150 ml of high purity distilled-in-glass methylene chloride was added followed by the remaining half portion of sample water. The methylene chloride prevents microbiological degradation and retards hydrolytic degradation of many organic components by removing them from the aqueous phase. A field blank was collected at each site in the same manner as a sample using distilled water (taken to each site from the laboratory) instead of waste or inlet water. All bottles were appropriately labelled and stored on ice.

Grab samples to be analyzed for volatile compounds were collected in 40 ml glass vials. Four samples were collected at both the inlet and outfall by filling each vial until it overflowed. This sampling method ensured that no air remained in the samples. The completely filled vials were sealed with screw-caps containing Teflon-lined silicon rubber septa and stored cap-side down on ice. A field blank consisting of distilled water was prepared at each site using the preceding overflow method. All water samples were stored at 4°C until they were extracted and/or analyzed by GC/MS.

SAMPLE ANALYSES

All sample analyses involved a GC/MS/COMP system that used high-resolution glass capillary GC columns. Volatile compounds were purged from water by helium, trapped on Tenax and subsequently desorbed. Semivolatile compounds were extracted from water with methylene chloride using an extraction scheme that gave the neutrals, acids, and bases as three separate fractions. These three fractions were analyzed by GC as well as by GC/MS/COMP.

INSTRUMENTATION

A Tekmar Liquid Sample Concentrator, Model LSC-1, was used for purging the volatile compounds. The device was equipped with a 25-ml sample container and the adsorbent tube was packed with 6 inches of 60/80 mesh Tenax GC. A 25-ml gas tight syringe with a 3-way valve and 12-inch needle was used to transfer the water samples to the LSC-1.

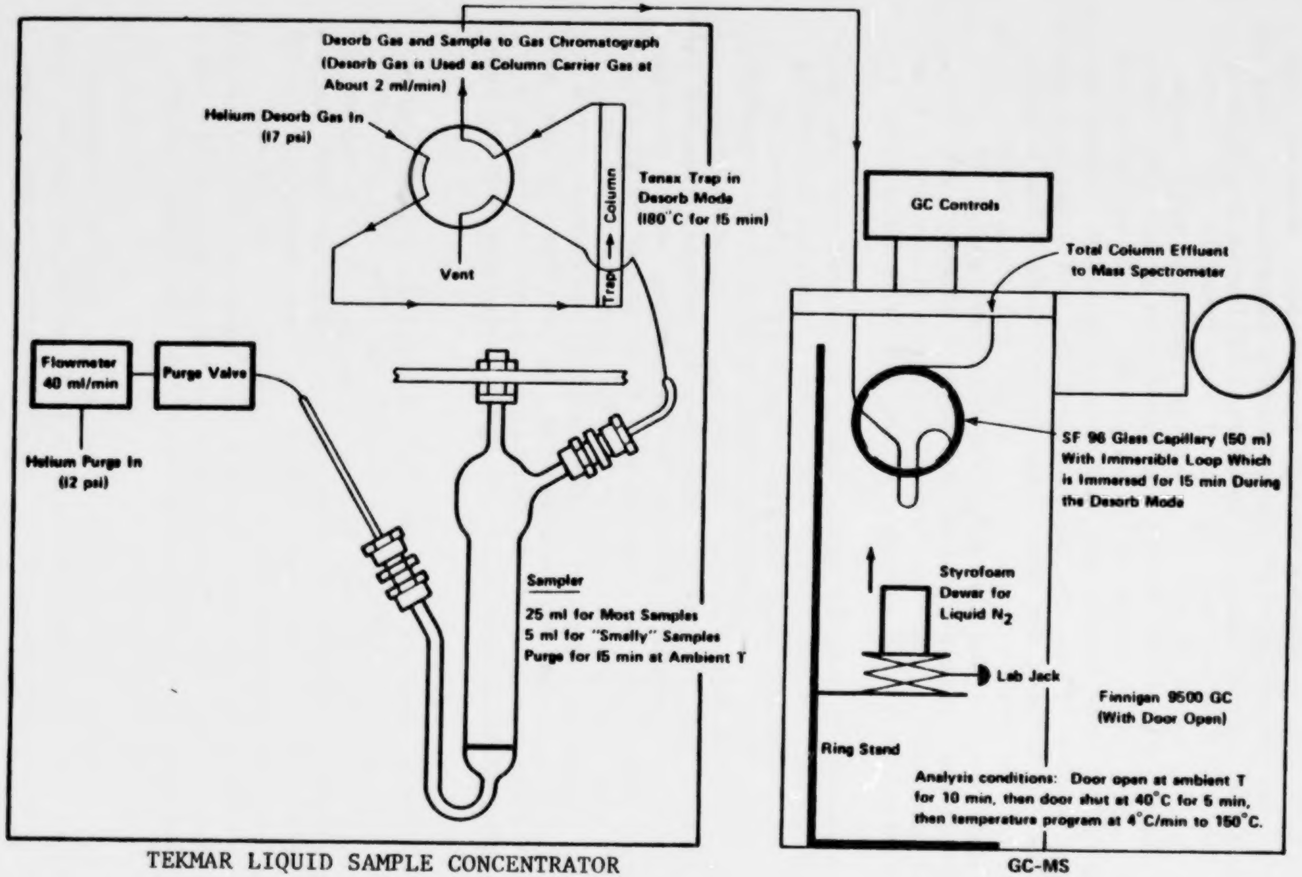
The GC/MS system for both the volatile and semivolatile analyses consisted of a Finnigan Model 9500 gas chromatograph coupled with a Finnigan Model 3200 quadrupole mass spectrometer. The mass spectrometer was interfaced to a Systems Industries Model 150 data system.

The GC column for volatile analyses was a 50 m x 0.25 mm i.d. glass capillary column (Perkin-Elmer) coated with SF-96 (a low molecular weight methyl silicone fluid). Figure 1 illustrates the instrumentation used in our purge and trap method.

The GC analyses of semivolatile compounds were performed using a Varian Model 1840 or Hewlett-Packard Model 5730 gas chromatograph equipped with a Hewlett-Packard automatic sampler. Each GC was fitted with a 30 m x 0.22 mm i.d. SE-30 glass capillary column (J. & W. Scientific). The calculation of retention index and concentration relative to the internal standard (pentadecylbenzene) was performed by a Spectra-Physics Model 4000 chromatography data system.

VOLATILE ANALYSIS PROCEDURES

During the course of this project it was mutually decided with the sponsor that all 85 samples would be analyzed for volatile compounds by using capillary column GC/MS instead of the usual packed column GC/MS system. The employment of capillary column GC/MS for routine volatile analyses proved to be a significant technical improvement in this project by providing well resolved GC peaks which result in clean mass spectra of volatile compounds.


Desorb Gas and Sample to Gas Chromatograph
(Desorb Gas is Used as Column Carrier Gas at
About 2 ml/min)
Helium Desorb Gas In
(17 psi)
Vent
Column
Trap
Tenax Trap in
Desorb Mode
(180°C for 15 min)
Flowmeter
40 ml/min
Purge Valve
Helium Purge In
(12 psi)
Sampler
25 ml for Most Samples
5 ml for "Smelly" Samples
Purge for 15 min at Ambient T
GC Controls
Total Column Effluent
to Mass Spectrometer
SF 96 Glass Capillary (50 m)
With Immersible Loop Which
is Immersed for 15 min During
the Desorb Mode
Styrofoam
Dewar for
Liquid N$_2$
Lab Jack
Finnigan 9500 GC
(With Door Open)
Ring Stand
Analysis conditions: Door open at ambient T
for 10 min, then door shut at 40°C for 5 min,
then temperature program at 4°C/min to 150°C.

TEKMAR LIQUID SAMPLE CONCENTRATOR

GC-MS

FIGURE 1. INSTRUMENTATION FOR PURGE AND TRAP ANALYSIS

Experimental Method

Since the glass capillary column was attached directly to the mass spectrometer, cryogenic trapping was used to concentrate the entire volatile sample as a plug on the head of the column. Thus no compounds were pumped away with the helium by passing through a separator. However, this method did require some modification of the procedure described in "Sampling and Analysis Procedures for Screening of Industrial Effluents for Priority Pollutants".(1) One modification was the use of only Tenax in the adsorbent tube. If silica gel was added at the front of the absorbent tube, large amounts of water vapor were eluted during the desorption step. This water sometimes formed a plug in the glass capillary column. In a second modification, the LSC-1 Desorb Mode outlet was used as the capillary column carrier gas. The helium entered a "T" at the back of the LSC-1 and a small pressure regulator was installed between the Desorb and Purge inlets. The pressure was set at 15 psi for the Desorb inlet (i.e., 15 psi was the pressure at the head of the capillary column) and the purge regulator was set at 12 psi. The flow rate through the capillary column was about 3 ml/min. The first coil of the glass capillary column was fashioned into a U-tube about 4 cm deep which was immersed in liquid nitrogen during the desorption step.

To analyze a sample, 25.0 ml of water sample was poured into the gas-tight syringe followed by the addition of 200 μl of a solution containing 200 ng of the internal standard (the internal standard was prepared by diluting 74 μl (100 mg) of 1,2,3-trichloropropane to 10.0 ml with methanol and then diluting 10 μl of this solution containing 100 μg of internal standard to 100 ml with sparged water); this gives an internal standard concentration of 8 μg/l. The sample was added to the purging device through a septum and sparged for 15 min with helium at a flow rate of 40 ml per min. The Texax trap was then desorbed for 15 min at 180° with the capillary U-tube immersed in liquid nitrogen. The LSC-1 was then switched to the Purge mode, the liquid nitrogen was removed from the capillary column, and data acquisition started. A plug of air reached the source in the mass spectrometer in about three minutes followed by the separated organic components.

The GC/MS conditions were as follows: 1) the initial column temperature was 25°C and held at this temperature for 10 min after the solvent front (air) passed through the column; 2) the column was quickly heated to 40°C and held at this temperature for 5 min; 3) the column was then temperature programmed at 4°C/min to 130°C and held at the final temperature until all the volatile components eluted (usually 10-15 min); 4) the MS was scanned from m/e 40-350 with the sensitivity at 10^{-7} and the electron multiplier voltage at about -2.00 KV. Between each run the purging device was rinsed several times with sparged distilled water and the Tenax trap was baked out at 210°C for 15 minutes.

2-Bromo-1-chloropropane was initially used as the internal standard. However, experiments revealed that the 2-bromo-1-chloropropane was not completely resolved from toluene and also exhibited two isomer peaks on the

SF-96 capillary column. Consequently, 1,2,3-trichloropropane was used as the internal standard. The internal standard (200 ng) was added to each sample including the blanks and reference solutions. Retention times relative to 1,2,3-trichloropropane were calculated for each compound found in the samples. Figure 2 shows a typical RGC of the volatile components in an industrial wastewater samples.

Quantitation

The quantitation of each volatile compound using extracted ion currents of major ions of each compound would be time consuming (computer time) and costly. Therefore, it was mutually agreed with the sponsor that a semiquantitative estimation of the amount of each volatile component found would be adequate for this program. Relative peak heights of reference compounds (i.e., response factors) in the normalized total ion chromatogram (T.I.C.) were used to estimate the concentrations of each compound in the samples. The relative responses of acetone, diethyl ether, benzene, chlorobenzene, and o-xylene (compounds which appear in many of the industrial samples) were determined to be in a 20-fold range and depended upon the stripping efficiency of the procedure (related to compound solubility and volatility) and the ionization and chromatographic characteristics (polarity, molecular weight, etc.) of the compounds. For compounds identified in the samples, estimated relative response factors were used to estimate the approximate quantity of each compound. Initially, relative responses for a few samples could not be obtained because the sample components were so concentrated that the internal standard peak was not observed in the normalized TIC plot. Consequently, three additional internal standards (bromochloromethane, 2-bromo-1-chloropropane and 1,4-dichlorobutane) were added to all samples. This modification permitted reliable semi-quantification of the volatile compounds in the industrial water samples. Table 2 lists the relative responses of internal and external standards used in our semiquantification of volatile compounds.

SEMIVOLATILE ANALYSIS PROCEDURES

Each of the 85 water samples was extracted to give three fractions containing the neutral, acidic, and basic semivolatile compounds, respectively. These fractions were gas chromatographed (methylated acid fraction) to obtain semiquantitative data and to prioritize the respective fractions for subsequent GC/MS/COMP analysis. Only the top priority fractions (total of 89) were analyzed by GC/MS/COMP.

Experimental Method

Semivolatile organic compounds were extracted from each water sample using the procedure illustrated in Figure 3.

Each 1500 ml sample, previously treated with 5 g of $KHSO_4$ and 75 g of NaCl, was spiked with three internal standards--hexaethylbenzene, 2,4-dimethylaniline and palmitic acid. The pH was adjusted to pH≈1 using H_2SO_4 and the sample extracted three times with nanograde distilled in glass

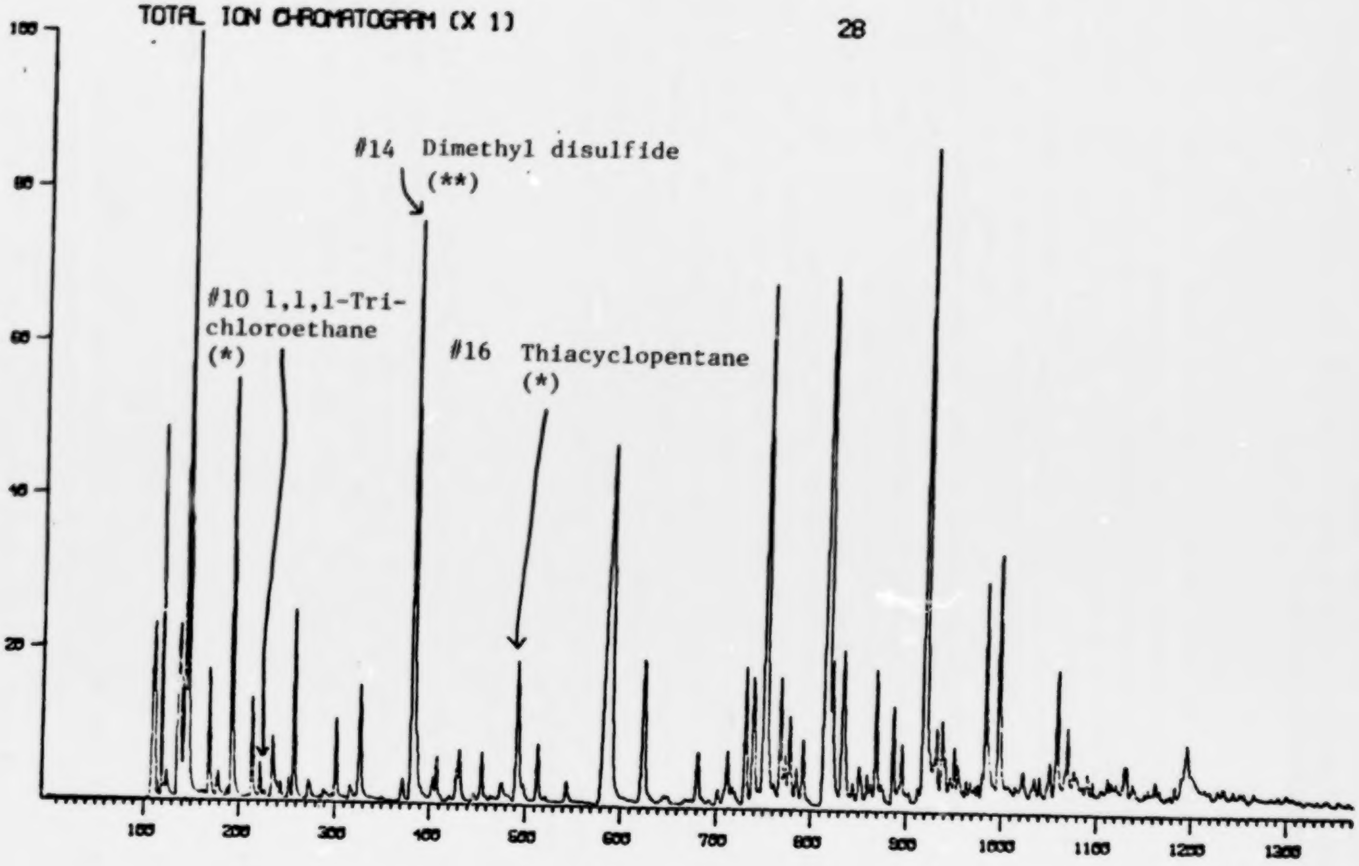


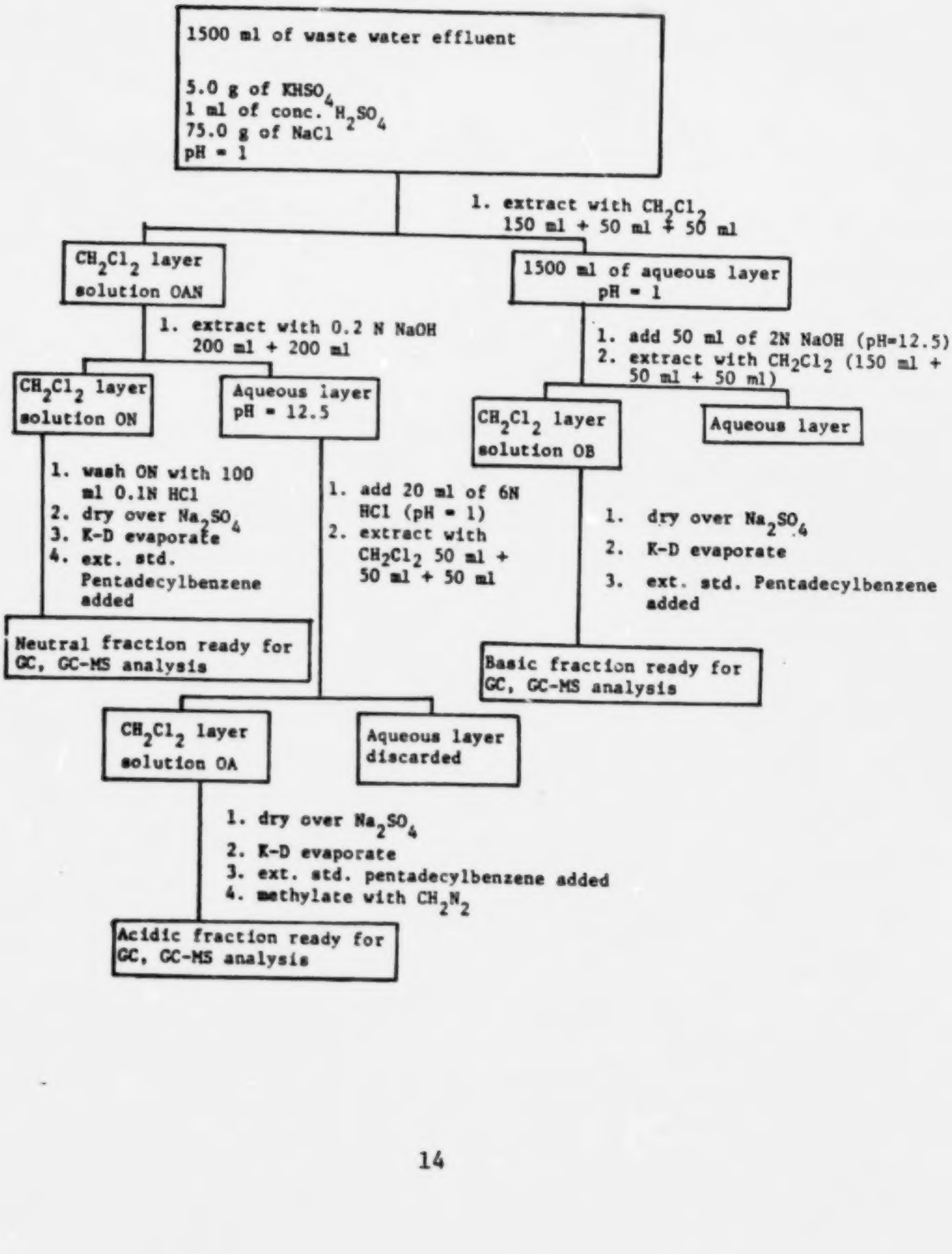
Figure 2. Total ion chromatogram of volatile fraction of industrial effluent.

TABLE 2. INTERNAL STANDARDS AND EXTERNAL STANDARDS

Compound	Amount in 25-ml water sample, ng	Concentration, μg/l	Relative Response[a]
Acetone	473	19.0	0.8
Diethyl ether	142	5.7	7.3
Benzene	178	7.0	11.5
Chlorobenzene	221	8.8	3.2
o-Xylene	176	7.0	3.8
Bromochloromethane	200	8.0	5.0
2-Bromo-1-chloropropane	200	8.0	3.9
1,4-Dichlorobutane	200	8.0	1.1
1,2,3-Trichloropropane	200	8.0	1.0

(a) Response/concentration relative to that of the internal standard, 1,2,3-Trichloropropane

FIGURE 3. EXTRACTION PROCEDURE


1500 ml of waste water effluent
5.0 g of $KHSO_4$
1 ml of conc. H_2SO_4
75.0 g of NaCl
pH = 1
1. extract with CH_2Cl_2 150 ml + 50 ml + 50 ml
CH_2Cl_2 layer solution OAN
1500 ml of aqueous layer pH = 1
1. extract with 0.2 N NaOH 200 ml + 200 ml
1. add 50 ml of 2N NaOH (pH=12.5)
2. extract with CH_2Cl_2 (150 ml + 50 ml + 50 ml)
CH_2Cl_2 layer solution ON
Aqueous layer pH = 12.5
CH_2Cl_2 layer solution OB
Aqueous layer
1. wash ON with 100 ml 0.1N HCl
2. dry over Na_2SO_4
3. K-D evaporate
4. ext. std. Pentadecylbenzene added
1. add 20 ml of 6N HCl (pH = 1)
2. extract with CH_2Cl_2 50 ml + 50 ml + 50 ml
1. dry over Na_2SO_4
2. K-D evaporate
3. ext. std. Pentadecylbenzene added
Neutral fraction ready for GC, GC-MS analysis
Basic fraction ready for GC, GC-MS analysis
CH_2Cl_2 layer solution OA
Aqueous layer discarded
1. dry over Na_2SO_4
2. K-D evaporate
3. ext. std. pentadecylbenzene added
4. methylate with CH_2N_2
Acidic fraction ready for GC, GC-MS analysis

methylene chloride. The combined methylene chloride extracts (neutral and acidic fractions) were extracted twice with 0.2N NaOH resulting in organic (neutral fraction) and aqueous (acidic fraction) layers. The organic layer was washed with 0.1N HCl, dried over anhydrous sodium sulfate, filtered, and concentrated to 400 µl using a Kuderna-Danish evaporator.

The aqueous layer (acidic fraction) was made acidic (pH≈1) with 6N HCl and extracted three times with methylene chloride. The resulting organic layer was dried, filtered and concentrated to 400 µl. The solution was split in half. Half was methylated using a diazomethane generator and the other half was stored for possible reanalysis.

The original acidic aqueous layer (basic fraction) was made alkaline, (pH≈12.5) using 2N NaOH, extracted three times with methylene chloride, dried, filtered, and concentrated to 400 µl.

An internal standard, 20 µg of pentadecylbenzene was added to each of the respective fractions together with 400 µl of benzene. Each fraction was concentrated to 400 µl, split in half and stored at 4°C until GC or GC/MS analysis. By replacing methylene chloride with the higher boiling solvent benzene, samples had longer storage life. More importantly, the "solvent effect" produced by benzene improved column resolution and peak shape in subsequent splitless injections of GC/MS analyses.

All 255 fractions were analyzed by GC using the conditions listed in Table 3.

TABLE 3. GAS CHROMATOGRAPHIC CONDITIONS*

Injection procedure	2 µl 10:1 split
Initial temperature	60°C
Initial time	5.0 min.
Programming rate	4°C/min.
Final temperature	260°C
Final time	35 min.
Injector temperature	250°C
Detector temperature	300°C

*30 m x 0.22 mm i.d. SE-30 glass capillary column.

Figures 4, 5 and 6 illustrate typical gas chromatograms of the respective neutral, acidic, and basic fractions from industrial waste-water effluents. The GC/MS conditions for semivolatile compound analysis were similar except that a 2 µl splitless injection was used.

Quantitation

The emphasis of this program was on the identification and not quantification of organic compounds. Consequently, semiquantitative methods based solely on gas chromatography were sufficient. The Spectra-Physics 4000 data

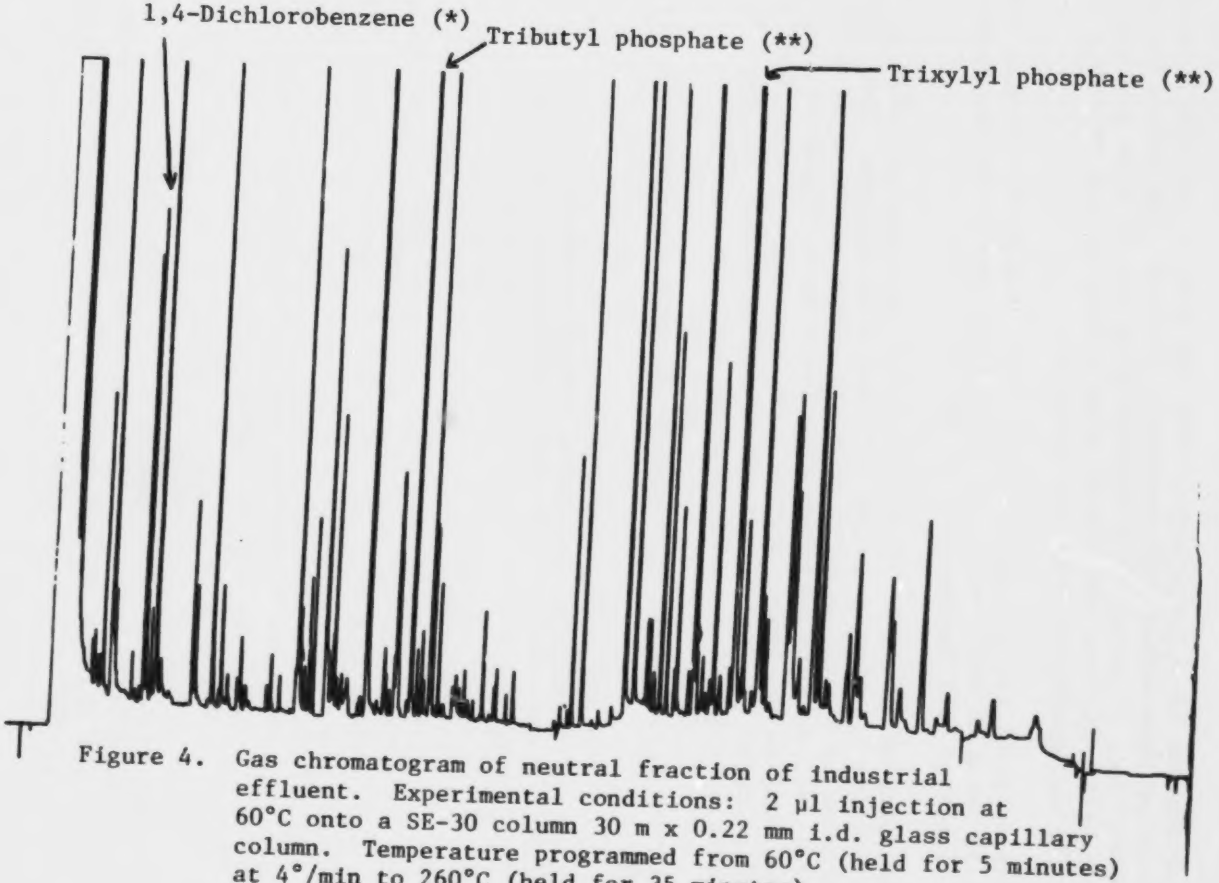


Figure 4. Gas chromatogram of neutral fraction of industrial effluent. Experimental conditions: 2 µl injection at 60°C onto a SE-30 column 30 m x 0.22 mm i.d. glass capillary column. Temperature programmed from 60°C (held for 5 minutes) at 4°/min to 260°C (held for 35 minutes).

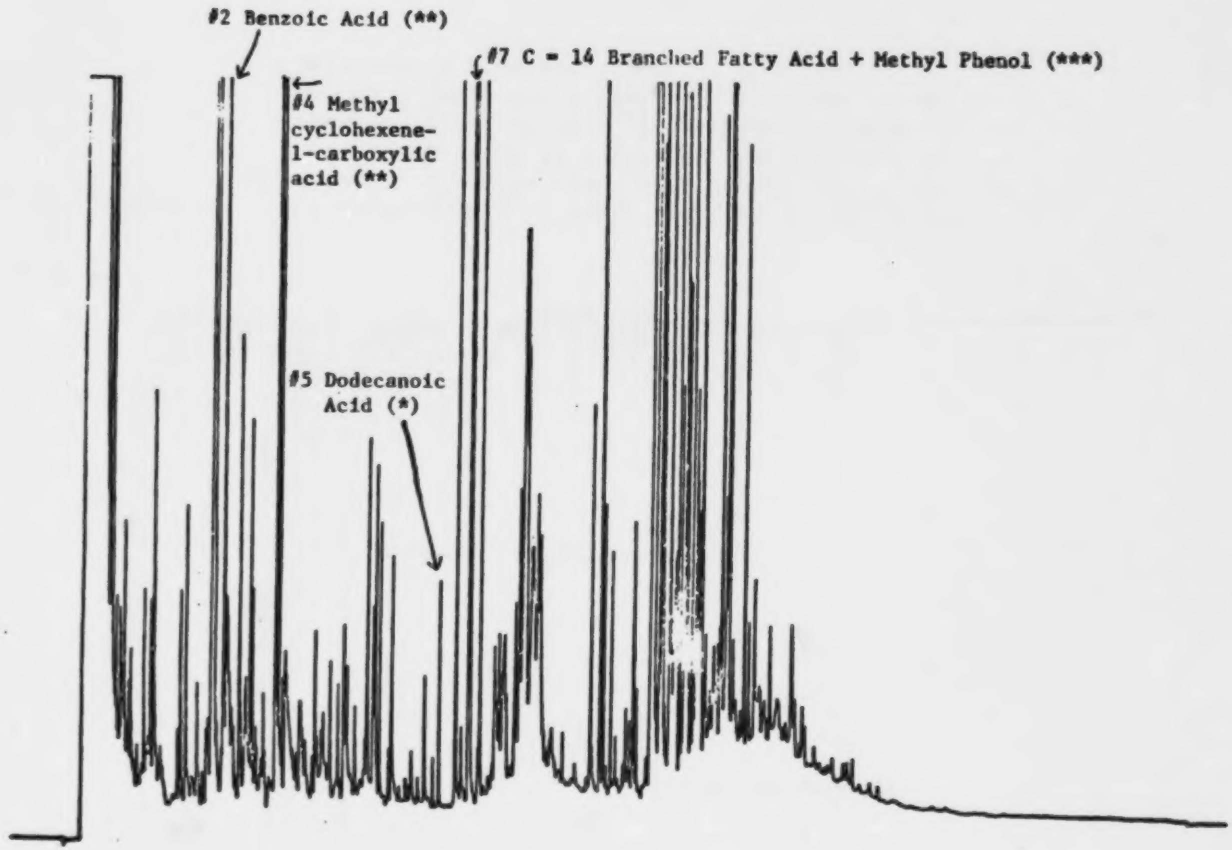


Figure 5. Gas chromatogram of acidic fraction of industrial effluent. Experimental conditions: 2 µl injection at 60°C onto a SE-30 column 30 m x 0.22 mm i.d. glass capillary column. Temperature programmed from 60°C (held for 5 minutes) at 4°/min to 260°C (held for 35 minutes).

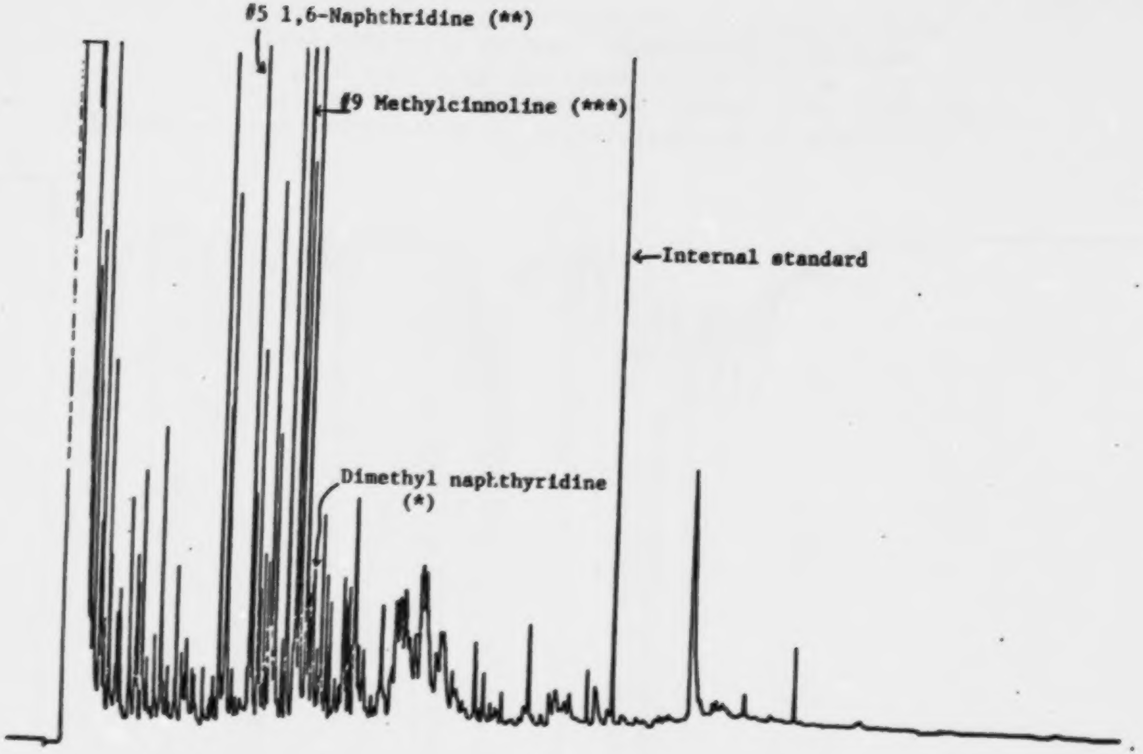


Figure 6. Gas chromatogram of basic fraction of industrial effluent. Experimental conditions: 2 µl injection at 60°C onto a SE-30 column 30 m x 0.22 mm i.d. glass capillary column. Temperature programmed from 60°C (held for 5 minutes) at 4°/min to 260°C (held for 35 minutes).

system calculated concentrations using pentadecylbenzene as an internal standard. The sample component concentrations were calculated using "estimated response factors" which were obtained by correlating the following:

(1) The relative response of a similar compound found in the BCL Standard Mixtures (Table 4);

(2) The recovery of the respective fractions (determined by comparison of internal with external standard);

(3) The shape of the respective GC peak and baseline (which indicated how accurately each peak area was integrated).

The reliability of our quantitative data depended ultimately upon the computer integration of the respective GC peak areas. Because of actual problems associated with this procedure (co-eluting compounds, poor GC peak shape and/or irregular baseline), the following ranges were established for reporting compound concentrations:

(1) * = less than 10 μg/l

(2) ** = 10-100 μg/l

(3) *** = greater than 100 μg/l.

QUALITY ASSURANCE STUDIES

An essential and enlightening aspect of this project was the continued use of various quality assurance measures. Because of the variety of chemical and physical properties of compounds expected to be found and the μg/l detection limit, stringent standards were necessary to validate our procedures for the extraction, detection, and identification of compounds from industrial wastewater effluents. These quality assurance standards included instrumental calibration, recovery studies, and process and field blank studies.

Gas Chromatograph Calibration

A standard solution containing 2,6-dimethylphenol (DMP), 2,4-dimethylaniline (DMA), decylaldehyde, decanol, _n_-tridecane, and _n_-tetradecane was injected into the GC to determine the polarity, separation number (SN), and number of effective plates (N_{eff}) of the glass capillary column. This evaluation was made each time a column was connected in the GC and each time column degradation was suspected. In order for a GC column to have been acceptable for sample analysis the following conditions had to be met.

(1) $N_{eff} \geq 50,000$

(2) $SN \leq 25$

(3) Area of DMP/Area of DMA = 0.5 to 2.0

Table 4. Recovery of Compounds in BCL Standard Mixture

Compound	No. of Runs	Recovery, %	Relative Standard Deviation, %
1. Chlorobenzene	4	94.3 ± 8.7	9.2
2. Nonane	4	87.9 ± 9.5	10.1
3. 1,2,4-Trimethylbenzene	4	98.9 ± 8.1	8.1
4. Naphthalene	4	88.4 ± 7.2	8.1
5. Decylaldehyde	4	88.7 ± 11.0	12.4
6. Dibenzofuran	4	93.0 ± 4.6	4.9
7. Tri-n-butyl Phosphate	4	85.8 ± 5.2	6.0
8. Pentadecanol	4	155.8 ± 60.8	39.0
9. Dibutyl Phthalate	4	85.1 ± 9.4	11.0
10. Carbazole	4	131.0 ± 12.9	9.8
11. Pyrene	4	88.6 ± 12.2	13.7
12. Methyl Stearate	4	82.8 ± 8.4	10.1
13. Heptadecylcyclohexane	4	79.0 ± 9.0	11.3
	Acidic Fraction		
1. 2,6-Dimethylphenol	5	97.5 ± 8.1	8.3
2. p-Nitrophenol	4	26.6 ± 3.4	12.7
3. m-Nitrobenzoic Acid	4	45.2 ± 20.4	45.0
4. 2,3,4,5-Tetrachlorophenol	5	97.0 ± 7.2	7.4
5. Palmitic Acid	5	118.8 ± 15.8	13.4
	Basic Fraction		
1. N-Ethylmorpholine	5	98.9 ± 8.4	8.4
2. Dibutylamine	2	70.5 ± 9.6	13.6
3. 2,4-Dimethylaniline	5	94.9 ± 14.4	15.1
4. Quinoline	5	109.5 ± 6.8	6.2
5. m-Nitroaniline	5	72.4 ± 11.8	16.3

(4) Width of half height for decanol $\leq$ 4 x width at half height for tridecane.

In addition, a mixture containing C_9 to C_{32} n-paraffins was analyzed periodically to calibrate the retention time in terms of retention index (R.I.). This retention index calibration was made each time a column was connected in the GC and each time the retention index of the internal standard changed by 4 units relative to the previously calibrated value. A typical gas chromatogram obtained by the injection of this calibration standard mixture is shown in Figure 7.

GC-MS-COMP Calibration and Evaluation

The GC-MS-COMP system is checked daily by injecting a tune-up standard mixture and employing the following procedures and criteria.

Mass Spectrometer Tune Up

(1) Adjust zero level of the mass spectrometer using a preamplifier setting 10^{-8} amp/volt, and the filament (800 μA) and electron multiplier (∿ 2kV, gain ∿5 x 10^4) on.

(2) Admit FC-43 into the ion source and tune the MS as follows:

(a) Using the potentiometers on the "Ion Source Controller", optimize the electronics to give highest intensity with best peak shape for m/e 219 as described by the manufacturer (see service manual).

(b) Set the controls to scan the range 400-600, and further adjust the ion source controller to give a 219 ion peak intensity of ∿50-70% of that of the repeller to ∿10 V, then decreasing the ion energy slightly. Again focus on m/e 219 and adjust the lens voltage for good peak shape. Tuning in this manner will favor the high mass end of the spectrum (i.e. >200). Decafluorotriphenylphosphine (DFTPP) is admitted via the solids probe into the mass spectrometer. Its spectrum should be comparable to that of Eichelberger, et al. [(Anal. Chem., 46 (7), 995 (1975)]. A spectrum of DFTPP taken in this manner is shown in Figure 8.

(c) Check peak shape and resolution at 18, 69, 219, 264, 414, and 502.

(d) Check calibration using CONT mode using 10 samples/amu.

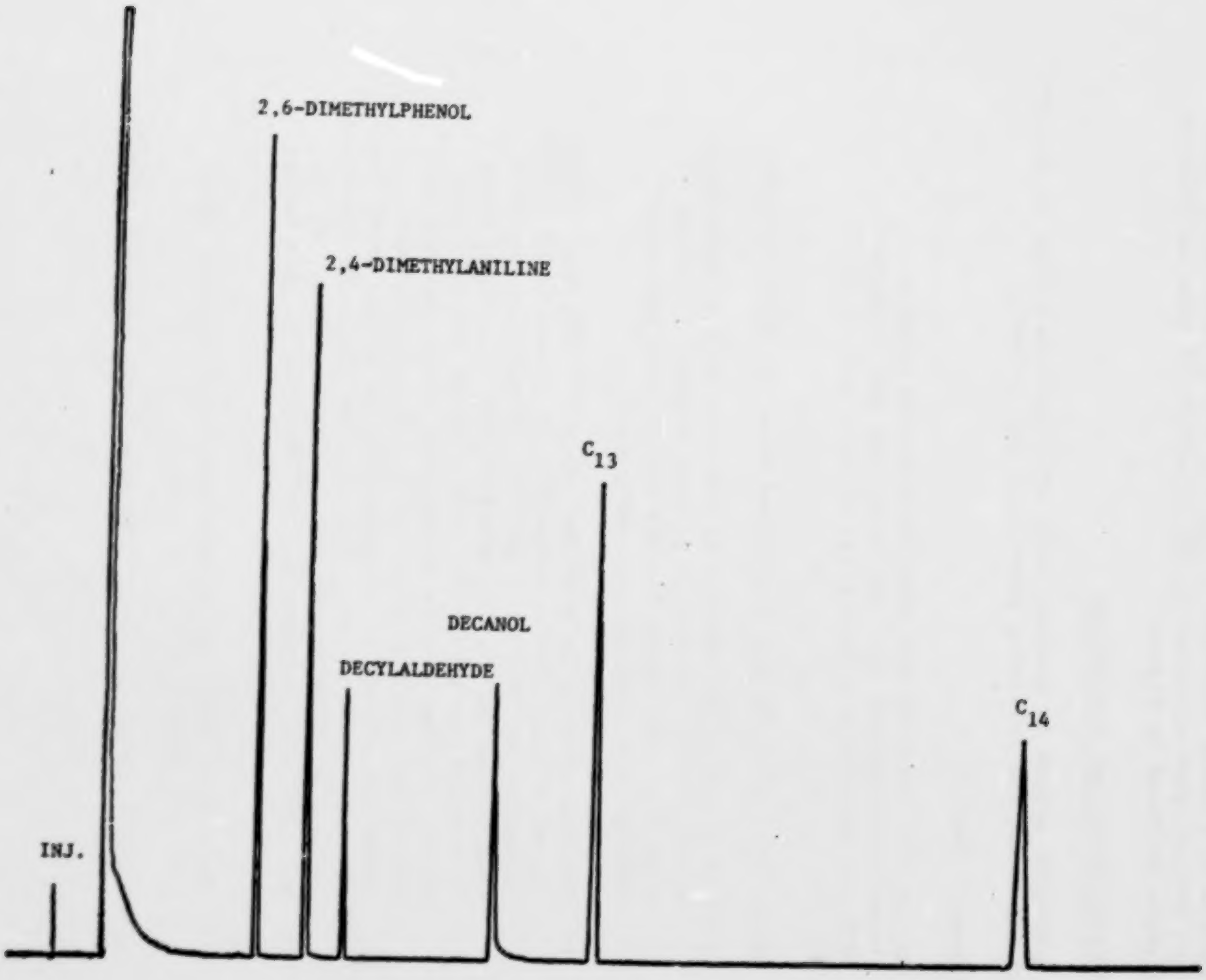


Figure 7. Glass capillary gas chromatogram of the calibration standard used for non-polar columns.

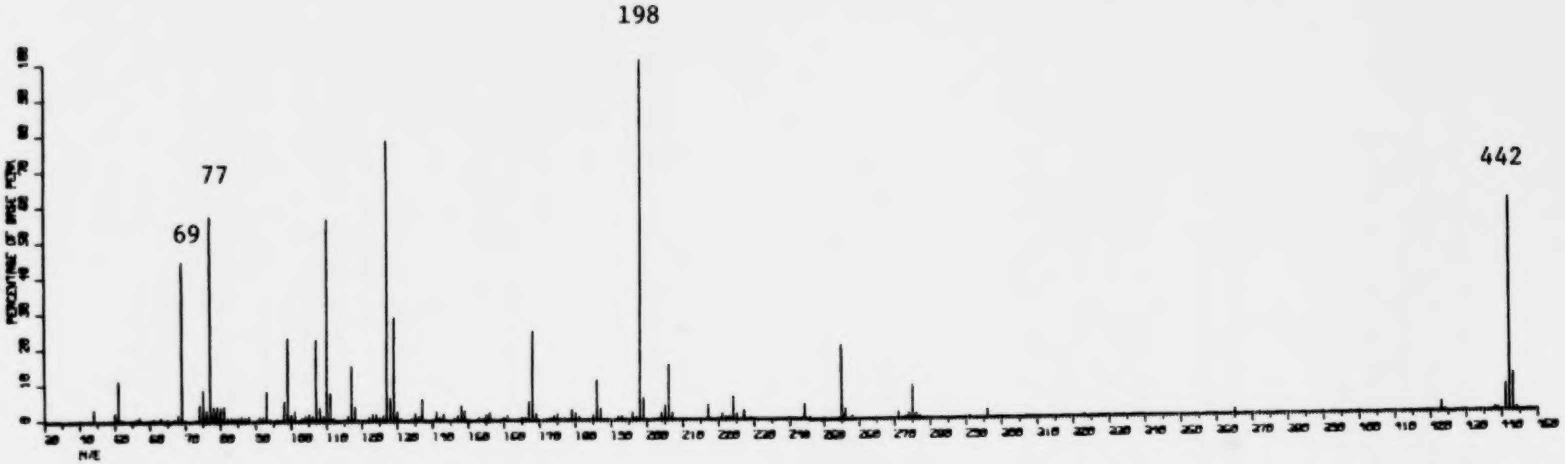


Figure 8. Electron impact mass spectrum of DFTPP

GC-MS Tune Up Mixture

Inject 1.0 µl of the "Tune Up Mixture" using a syringe with a 4" needle and splitless techniques. This mixture contains 30 ng each of 2,4-dimethylaniline and 2,6-dimethylphenol, and 10 ng each of 1-octadecene, octadecane, phytane, DFTPP, and methyl stearate. The conditions of the GC and computer are as follows:

(1) GC

- (a) Cool column to room temperature
- (b) Set initial temperature to 20°C and final temperature to 200°C
- (c) Set the program rate to 20°C/min
- (d) Inject 1.0 µl of the mixture using splitless techniques
- (e) When the solvent elutes into the mass spectrometer, begin the temperature program
- (f) Data collection can begin after solvent has passed

(2) Data System

- (a) Mode: IFSS
- (b) Max repeat count: 5
- (c) Integration time: 2
- (d) Check lower threshold: 2
- (e) Lower threshold: 3
- (f) Upper threshold: 1
- (g) Clock: Y
- (h) Fast scan opt: Y
- (i) Delay between scans: CR
- (j) Start clock 10 seconds after GC injection

GC-MS-Comp Evaluation

The resulting data were evaluated using the Selected Ion Summation Program (SIS) and plotting the Reconstructed Gas Chromatogram (RGC). A typical SIS reconstructed chromatogram is shown in Figure 9. The following parameters were evaluated:

(1) Capillary column pH - Peak heights of aniline (DMA) and phenol (DMP) were equal if the column was neutral; a decrease in aniline indicated an acidic column and a decrease in phenol indicated a basic column. Area of DMP/Area of DMA should be within the range of 0.5 to 2.0.

(2) Capillary column resolution - The hydrocarbon GC peaks were used to evaluate resolution. The GC peaks should be resolved with no more than a 50% valley.

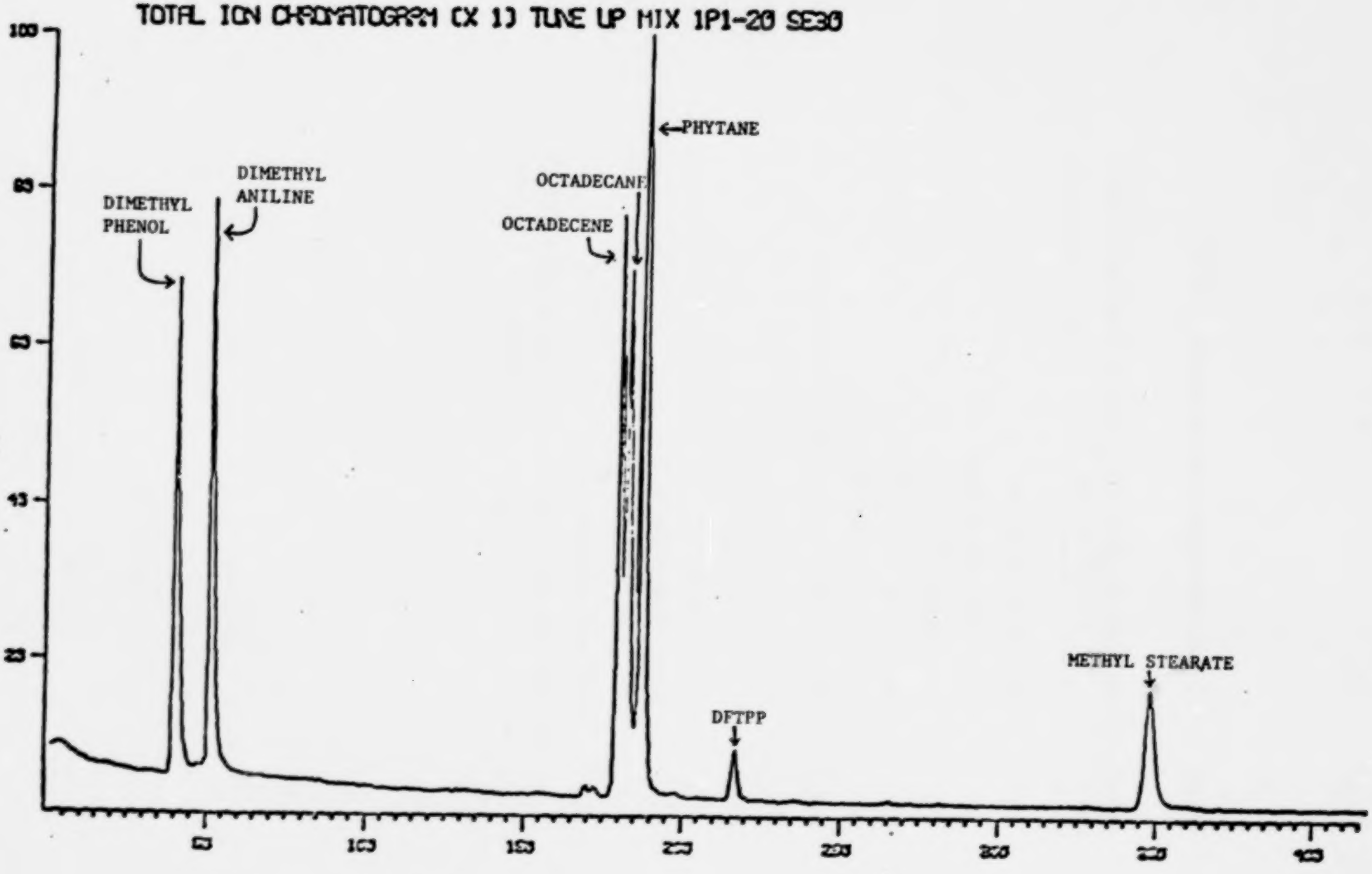


Figure 9. GC-MS-COMP tune up mixture chromatogram on a 30M SE30 capillary column

Table 5. Decafluorotriphenylphosphine (DFTPP)

Mass	Ion Abundance Criteria
51	30-60% of Mass 198
68	Less than 2% of Mass 69
70	Less than 2% of Mass 69
127	40-60% of Mass 198
197	Less than 1% of Mass 198
198	Base peak, 100% relative abundance
199	5-9% of Mass 198
275	10-30% of Mass 198
365	1% of Mass 198
441	Less than Mass 443
442	Greater than 40% of Mass 198
443	17-23% of Mass 442

Eichelberger, et al., Analytical Chemistry, 47 (7) 995 (1975).

(3) MS Tuning - DFTPP was used to evaluate the MS tuning under dynamic conditions. A spectrum on the front side of the DFTPP GC peak (before peak maximum if possible) was observed using CRTPLT. Eichelberger's criteria were used to evaluate this spectrum. A summary of these criteria are given in Table 5.

(4) GC/MS transfer line - Methyl stearate was included in the mixture to evaluate the transfer line system of the GC/MS. When the transfer line was inadequately heated, the methyl stearate peak tailed. Obtaining a symmetrical peak for methyl stearate verified that large, involatile molecules can elute from the capillary column into the mass spectrometer.

Recovery Studies

For the semivolatile compound recovery studies, 13 neutral compounds, 5 basic compounds and 5 acid compounds (BCL Standard Mixture, see Table 4) were selected to ensure a wide range of GC retention times and different functional groups. Recovery studies were performed by analysis of process blanks spiked with the BCL Standard Mixture at a level of 13.3 μg/l. Two process blanks were analyzed in one set of runs and three process blanks were analyzed in another set of runs one week later. Recovery data are given in Table 4. Representative gas chromatograms of neutral, basic and acidic process blanks are shown in Figures 10, 11 and 12, respectively.

For most compounds, recovery was greater than 80%. Coeluting contaminants accounted for excessively high recoveries for pentadecanol and carbazole. Two compounds, p-nitrophenol and m-nitrobenzoic acid gave low recoveries, 27% and 45%, respectively. This was expected since these two acid compounds are very polar and fairly soluble in water. The reproducibility of the recoveries achievable is indicated by relative standard deviations of less than 15% in most cases.

As is true for all analytical programs, a continuing quality assurance program is necessary to ensure continued reliability of data. Consequently, weekly recovery checks carried out over a period of 4 months were made for this program. Table 6 lists these results.

The periodic recoveries of each compound in the BCL standard mixture generally averaged over 70%. The reproducibility of the respective recoveries was indicated by relative standard deviations of approximately 20% in most cases. Only the polar compounds p-nitrophenol, m-nitrobenzoic acid and m-nitroaniline had low recoveries and/or high relative standard deviations.

Process and Field Blank Studies

Blank studies were performed on each of the following reagents used in the sample collection and extraction procedures: CH_2Cl_2, NaCl, $KHSO_4$, Na_2SO_4, 2N NaOH, 6N HCl, H_2O (millipore water). Methylene chloride was studied by 1000-fold concentration followed by GC analysis. All other reagents were extracted with CH_2Cl_2 which was then concentrated for GC analysis. Similar studies were carried out on the diazomethane generator, sample vials, filter paper, and Teflon liners (for vial caps). The GC results indicated that

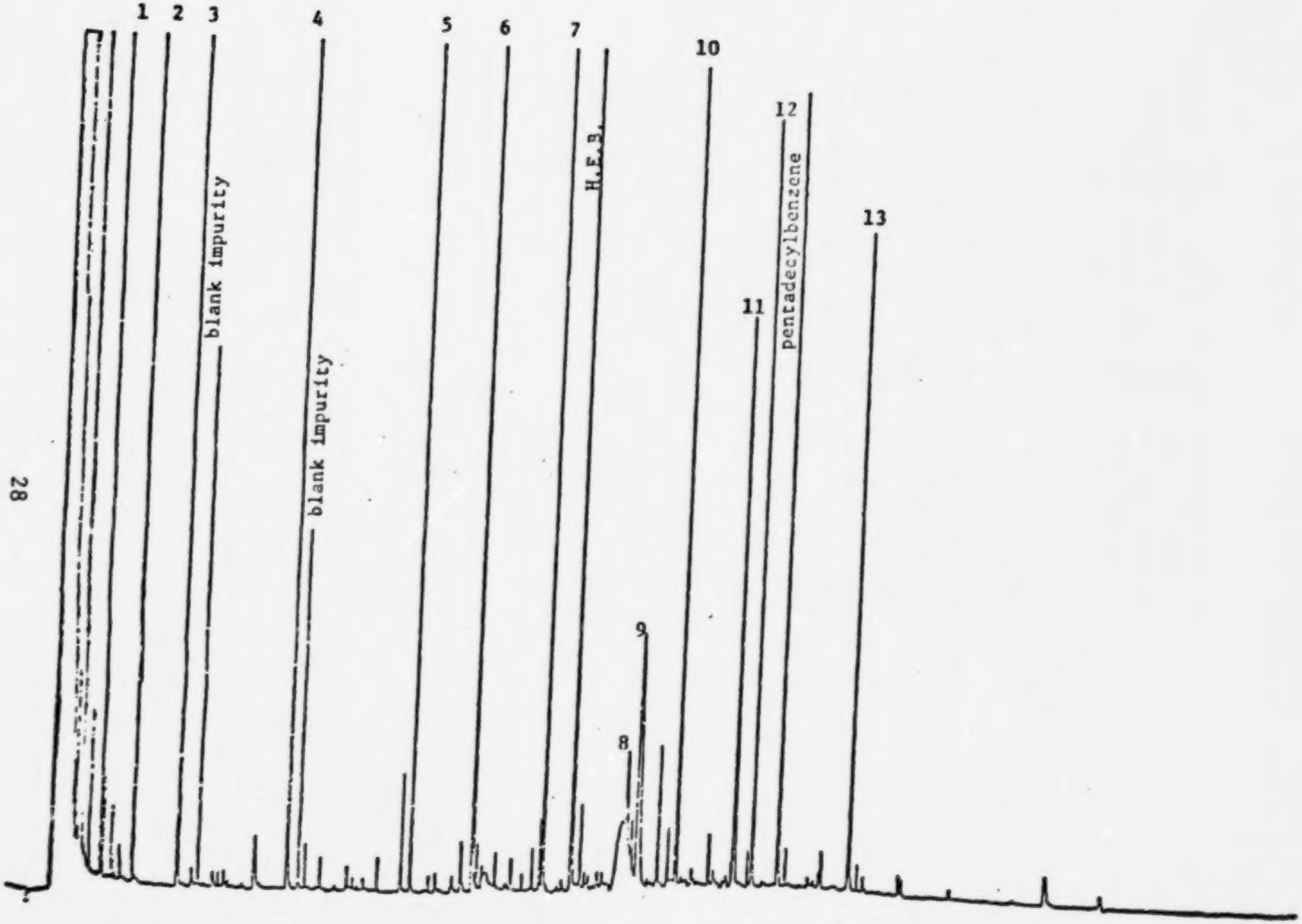


Figure 10. Gas chromatogram of neutral fraction from water spiked with BCL standard mixture

Experimental conditions: 2 µl injection at 60°C onto a SE-30 column 3 m x 0.22 mm i.d. glass capillary column. Temperature programmed from 60°C (held for 5 minutes) at 4°/min to 260°C (held for 35 minutes). See Table 4 for identity of components.

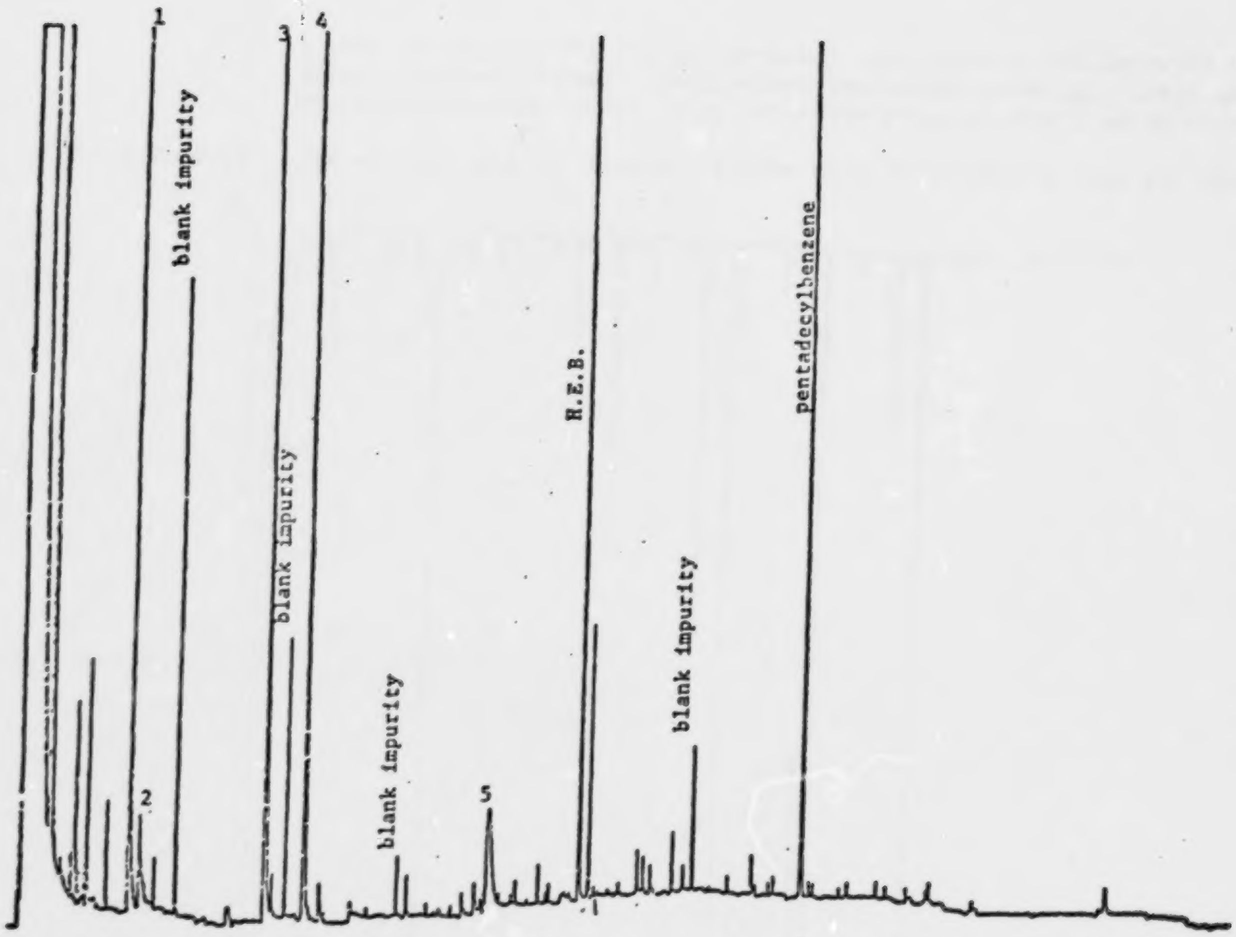


Figure 11. Gas chromatogram of basic fraction from water spiked with BCL standard mixture

Experimental conditions: 2 µl injection at 60°C onto a SE-30 column 30 m x 0.22 mm i.d. glass capillary column. Temperature programmed from 60°C (held for 5 minutes) at 4°/min to 260°C (held for 35 minutes). See Table 4 for identity of components.

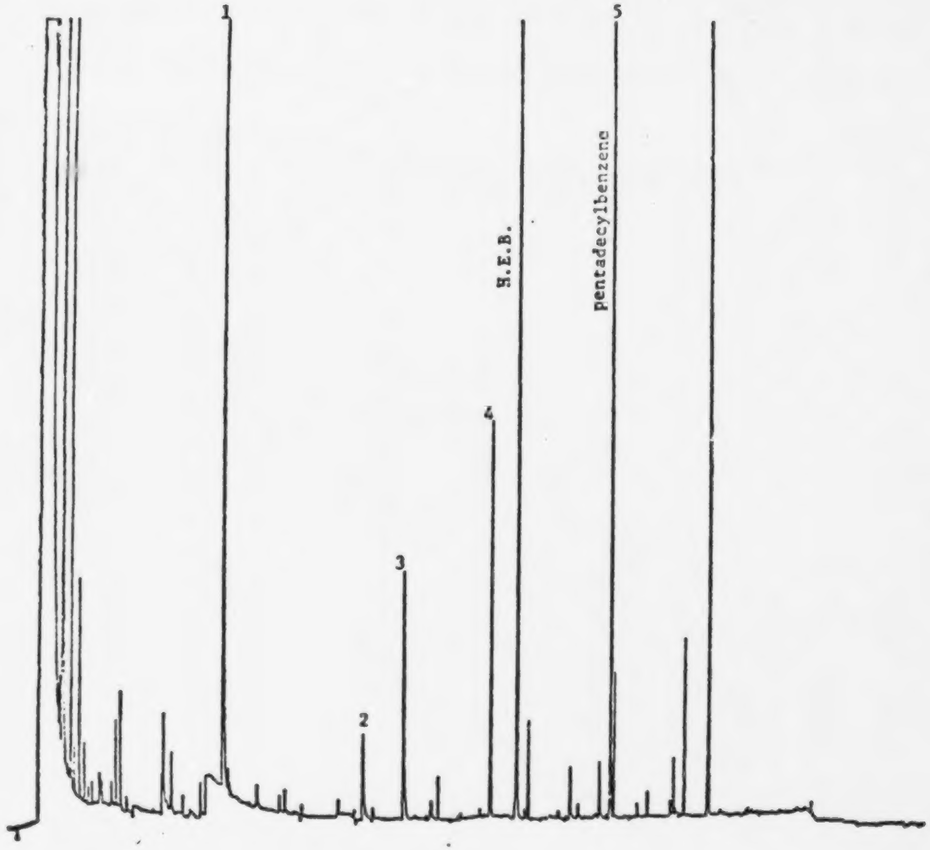


Figure 12. Gas chromatogram of acidic fraction from water spiked with BCL standard mixture

Experimental conditions: 2 µl injection at 60°C onto a SE-30 column 30 m x 0.22 mm i.d. glass capillary column. Temperature programmed from 60°C (held for 5 minutes) at 4°/min to 260°C (held for 35 minutes). See Table 4 for identity of components.

Table 6. Periodic recovery of compounds in BCL standard mixture

Compound	Recovery, %, From Spiked Process Blank Extracted on Given Date								
	12/27/77	1/3/78	1/11/78	1/23/78	1/31/78	2/6/78	2/9/78	2/13/78	2/20/78
Neutral Fraction									
1. Chlorobenzene	111	96.2	105	57.6	83.6	67.9	108.2	69.2	72.3
2. Nonane	106	95.5	96.0	50.5	74.4	55.6	80.9	26.3	60.9
3. 1,2,4-Trimethylbenzene	115	107	106	72.3	58.4	48.0	94.1	53.3	75.8
4. Naphthalene	108	99.5	108	87.9	74.9	73.1	104	81.8	80.2
5. Decylaldehyde	108	93.1	107	101	86.6	78.6	30.1	40.1	86.8
6. Dibenzofuran	116	105	114	103	71.5	76.7	98.1	105	84.9
7. Tri-n-butyl phosphate	108	85.4	118	110	104	118	98.7	125	82.5
8. Pentadecanol	114	125	106	118	109	115	69.5	104	80.0
9. Dibutyl phthalate	102	76.2	125	99.5	118	129	73.3	111	96.7
10. Carbazole	112	88.7	116	106	77.1	91.9	79.7	115	140
11. Pyrene	80.0	79.1	95.2	105	75.5	90.1	72.2	101	77.5
12. Methyl stearate	86.6	82.5	104	101	89.2	108	74.4	108	105
13. Heptadecylcyclohexane	76.0	71.3	96.4	98.8	78.3	84.1	78.3	81.2	84.4
14. Hexamethylbenzene	--	--	--	104	85.1	121	113	116	93.1
Acidic Fraction									
1. 2,6-Dimethylphenol	57.5	51.9	33.3	62.5	94.1	81.6	68.3	59.5	70.1
2. p-Nitrophenol	16.7	10.7	21.0	20.3	35.6	12.5	29.8	24.6	21.3
3. m-Nitrobenzoic acid	14.4	16.6	9.1	40.0	37.5	10.2	28.0	57.5	36.0
4. 2,3,4,5-Tetrachlorophenol	74.4	70.0	55.8	56.6	75.8	66.7	60.6	70.1	63.1
5. Palmitic acid	86.9	75.4	74.5	62.1	85.5	71.4	57.1	74.6	71.4
Basic Fraction									
1. N-ethylmorpholine	78.7	88.9	106	75.9	94.1	61.2	69.4	42.9	66.4
2. Dibutylamine	107	125	128	75.6	74.4	82.5	58.2	52.1	101
3. 2,4-Dimethylaniline	68.1	81.8	90.9	92.1	76.9	88.1	111	92.1	107
4. Quinoline	82.9	88.6	107	107	121	95.6	109	85.7	110
5. m-Nitroaniline	30.0	20.9	15.0	49.0	63.0	46.2	68.7	15.1	32.0

Table 6. (Continued)

Compound	Recovery, %, From Spiked Process Blank Extracted on Given Date 3/15/78	3/20/78	3/27/78	4/1/78	4/10/78	4/17/78	Avg. ± Std. Dev. (%)	Relative Std. Dev. (%)
Neutral Fraction								
1. Chlorobenzene	73.6	65.3	51.5	85.7	69.4	61.2	78.5 ± 18.3	23.3
2. Nonane	82.6	73.8	55.0	61.7	60.1	86.9	71.1 ± 20.5	28.8
3. 1,2,4-Trimethylbenzene	94.1	82.2	68.8	92.1	84.1	109	84.0 ± 20.8	24.8
4. Naphthalene	93.1	80.0	73.8	68.3	59.2	63.3	83.8 ± 15.3	18.2
5. Decylaldehyde	80.5	82.4	69.1	53.7	60.2	57.9	75.7 ± 22.8	30.1
6. Dibenzofuran	88.8	83.6	93.2	95.3	54.2	50.8	89.3 ± 19.0	21.2
7. Tri-n-butyl phosphate	93.2	84.3	80.8	96.7	56.7	47.2	93.9 ± 21.2	22.5
8. Pentadecanol	102	79.3	80.3	48.5	42.2	37.5	86.6 ± 27.8	32.0
10. Carbazole	87.3	75.0	96.4	53.3	61.7	55.3	90.3 ± 23.8	26.4
11. Pyrene	76.6	68.2	73.4	55.6	61.1	57.1	77.8 ± 14.3	18.4
12. Methyl stearate	82.6	72.6	78.3	57.1	52.1	47.5	83.3 ± 19.4	23.2
13. Heptadecylcyclohexane	84.6	86.6	75.2	55.1	56.2	53.1	77.3 ± 13.3	17.2
14. Hexamethylbenzene	101	70.1	101	76.4	73.6	96.4	95.9 ± 16.3	17.0
Acidic Fraction								
1. 2,6-Dimethylphenol	75.1	75.0	96.7	55.1	83.3	53.3	67.8 ± 16.5	24.3
2. p-Nitrophenol	38.3	27.7	23.4	21.2	27.7	23.4	23.6 ± 7.3	20.9
3. m-Nitrobenzoic acid	46.0	40.0	44.0	19.0	14.0	16.1	28.5 ± 14.9	52.2
4. 2,3,4,5-Tetrachlorophenol	75.8	66.7	84.8	42.4	72.7	40.0	66.0 ± 11.9	18.0
5. Palmitic acid	74.6	74.3	71.5	44.3	65.7	41.0	68.7 ± 12.6	18.3
Basic Fraction								
1. n-Ethylmorpholine	88.0	92.5	88.0	120	108	80.0	84.0 ± 19.0	22.6
2. Dibutylamine	73.0	69.9	73.2	80.9	40.2	55.2	79.7 ± 24.8	30.1
3. 2,4-Dimethylaniline	85.0	68.3	66.7	123	96.4	64.3	87.4 ± 16.7	19.1
4. Quinoline	98.8	72.6	82.1	90.5	112	71.8	95.6 ± 14.5	15.2
5. m-Nitroaniline	31.4	20.1	28.6	40.0	40.2	14.3	34.2 ± 16.5	48.2

no contaminants from these sources were present at levels equivalent to <1 µg/l of water analyzed. Figures 13, 14, and 15 show typical examples of neutral, basic, and acidic process blanks, respectively.

Volatile sample blanks were generally run at the beginning of each day's analyses. The water used was previously sparged overnight with 50 ml/min of nitrogen at 50°C. The sparged water blanks generally yielded several small peaks (<1 µg/l) which probably are contaminants in the commercial distilled water. Figures 16, 17, and 18 show volatile sample process blanks and water spiked with internal and external standards.

Field blanks were obtained for each site sampled. Analysis of various field blanks for volatile and semivolatile compounds indicated no significant contamination occurred during any of our sampling procedures. Methylene chloride and chloroform were found in many of the volatile field blanks but at levels below the concentrations found in the respective effluent samples.

PRIORITY CRITERIA FOR GC/MS ANALYSES

In an effort to obtain as much useful information as possible within a limited budget it was mutually agreed with the sponsor that GC/MS analysis of semivolatiles would be performed only on selected fractions. Priority was given to those fractions which were shown by GC analysis to contain several components at levels higher than 10 µg/liter that could not be tentatively identified on the basis of their GC patterns and retention indices. Table 7 lists the three priority ratings and their respective criteria. In most cases, only the "++" rated fractions were analyzed by GC/MS. In total, 89 fractions (39 neutrals, 29 acidics and 21 basics) were analyzed by GC/MS.

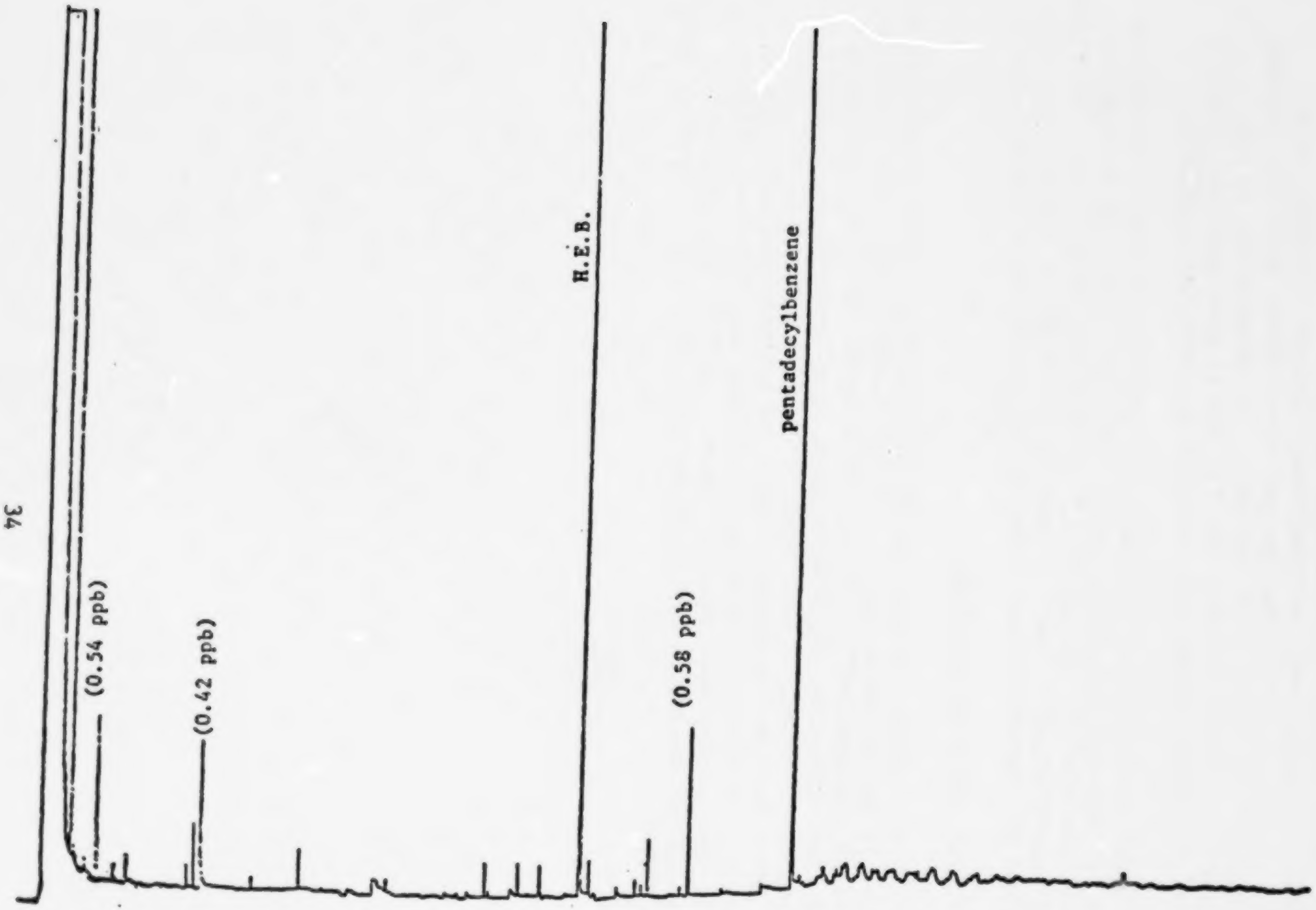


Figure 13. Neutral fraction process blank

Experimental conditions: 2 μl injection at 60°C onto a SE-30 column 30m x 0.22 mm i.d. glass capillary column. Temperature programmed from 60°C (held for 5 minutes) at 4°/min to 260°C (held for 35 minutes).

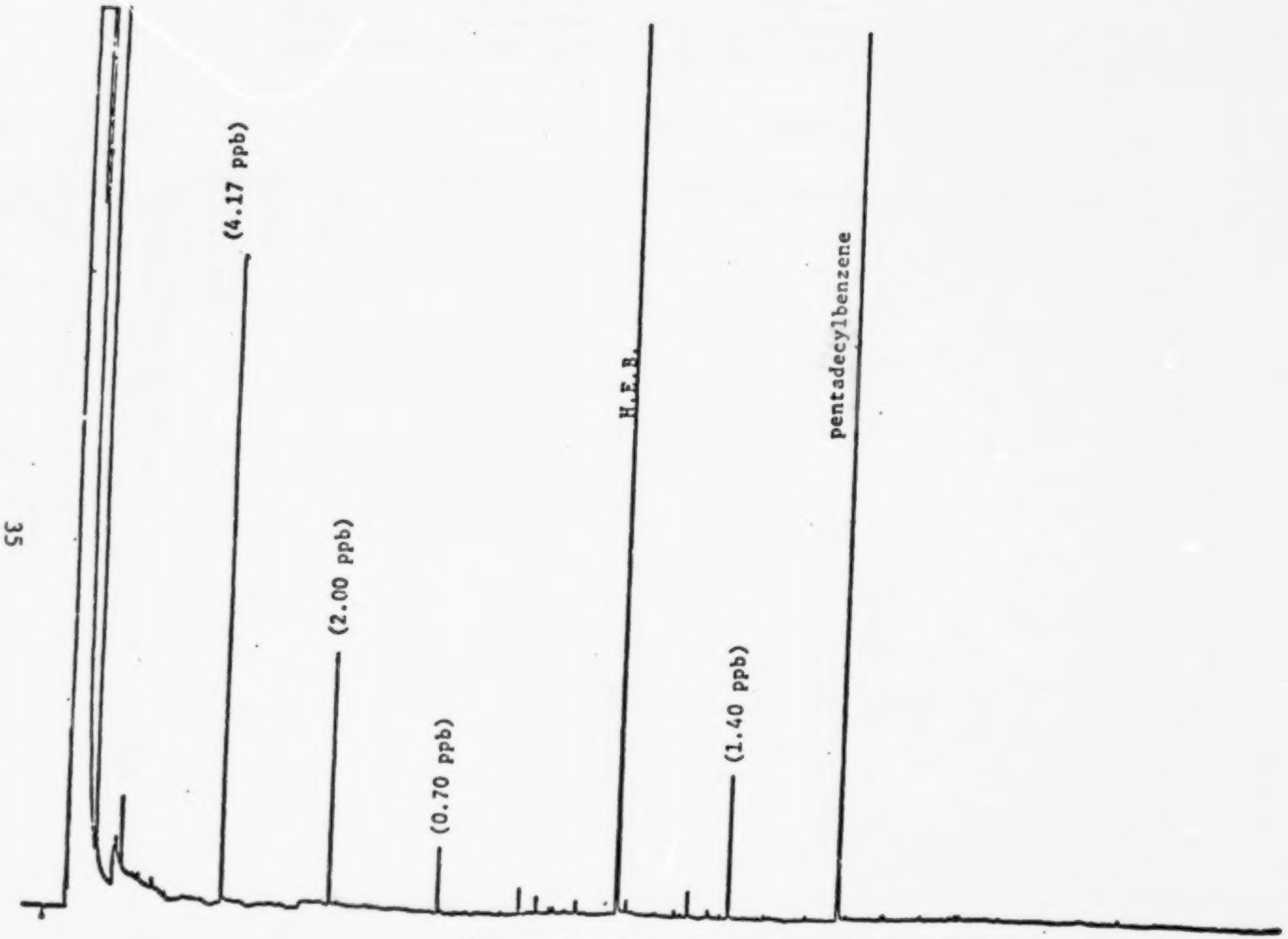


Figure 15. Basic fraction process blank

Experimental conditions: 2 µl injection at 60°C onto a SE-30 column 30 m x 0.22 mm i.d. glass capillary column. Temperature programmed from 60°C (held for 5 minutes) at 4°/min to 260° (held for 35 minutes).

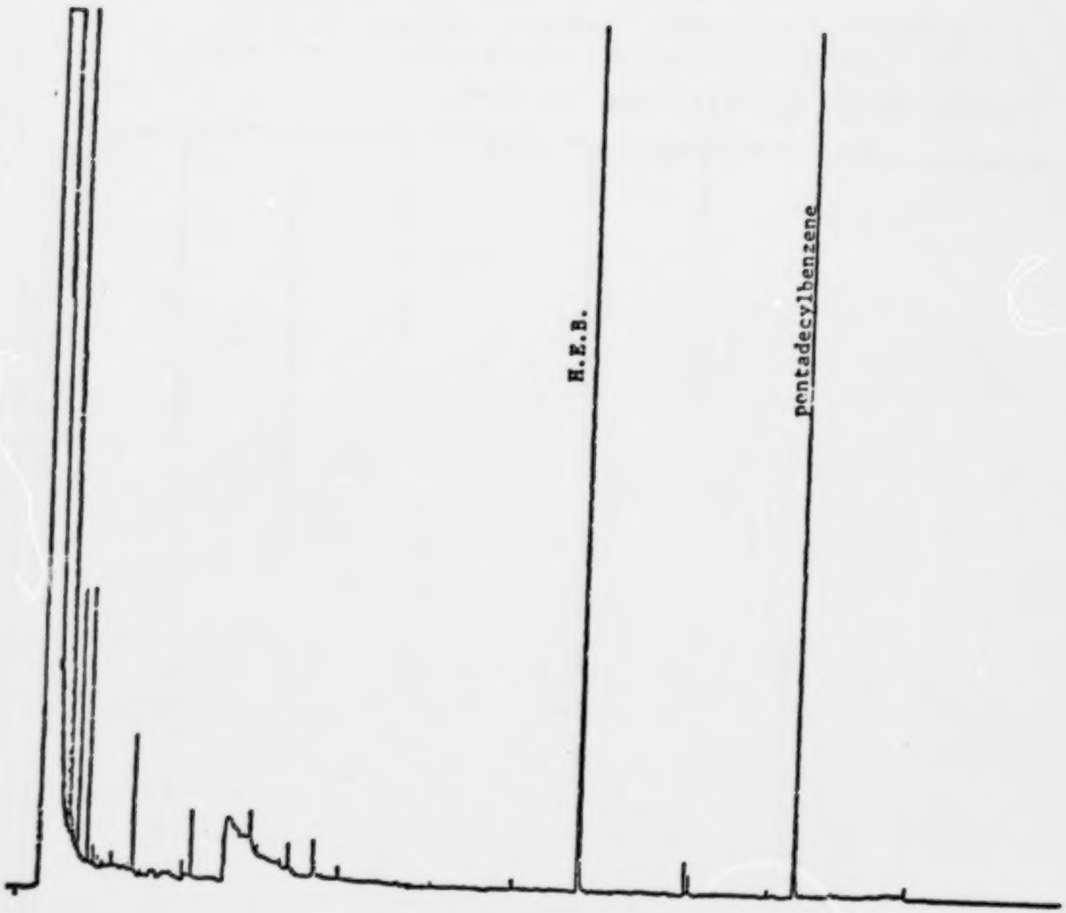


Figure 15. Acidic fraction process blank

Experimental conditions: 2 µl injection at 60°C onto a SE-30 column 30 m x 0.22 mm i.d. glass capillary column. Temperature programmed from 60°C (held for 5 minutes) at 4°/min to 260°C (held for 35 minutes).

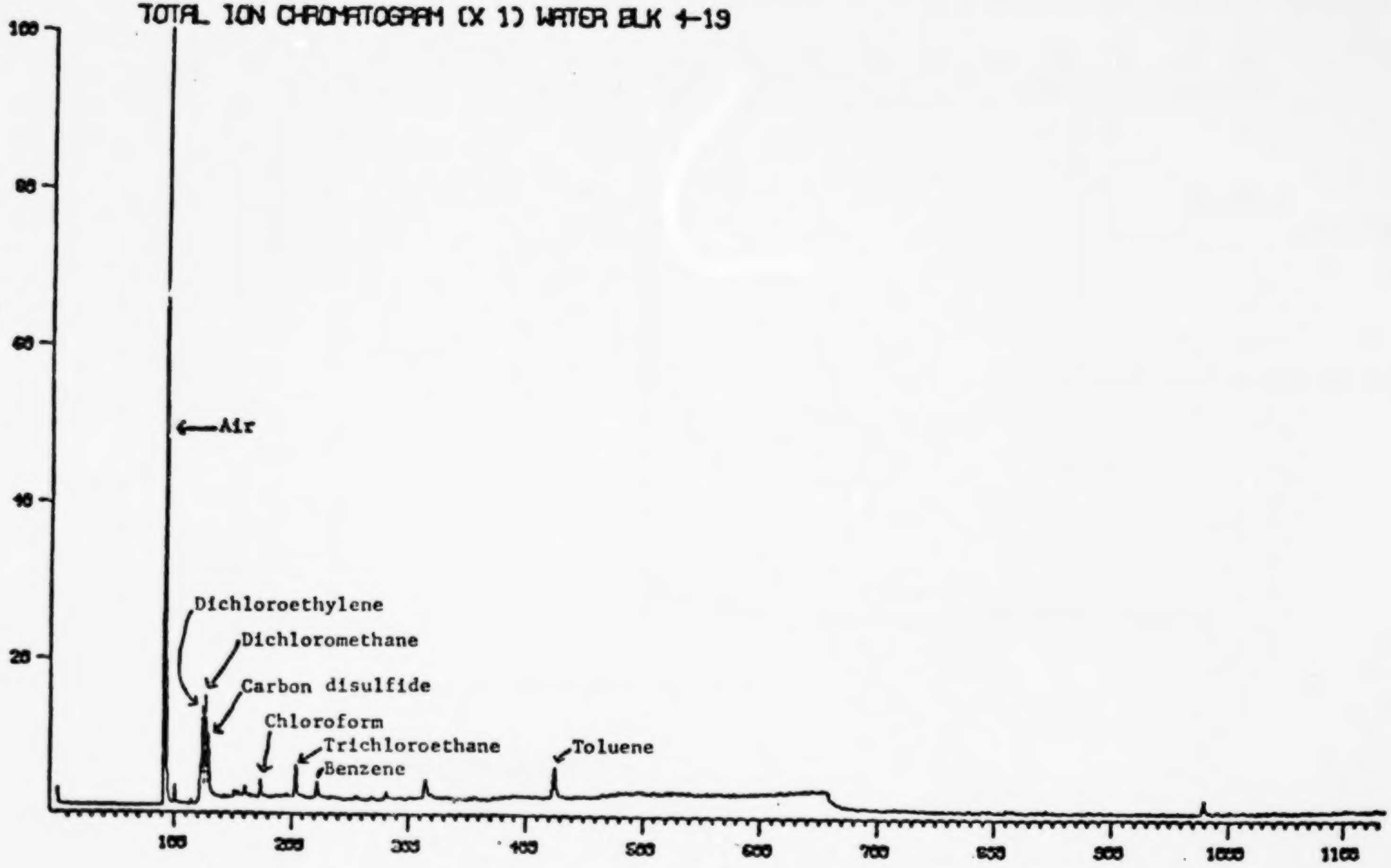


Figure 16. Total ion chromatogram obtained from water blank.

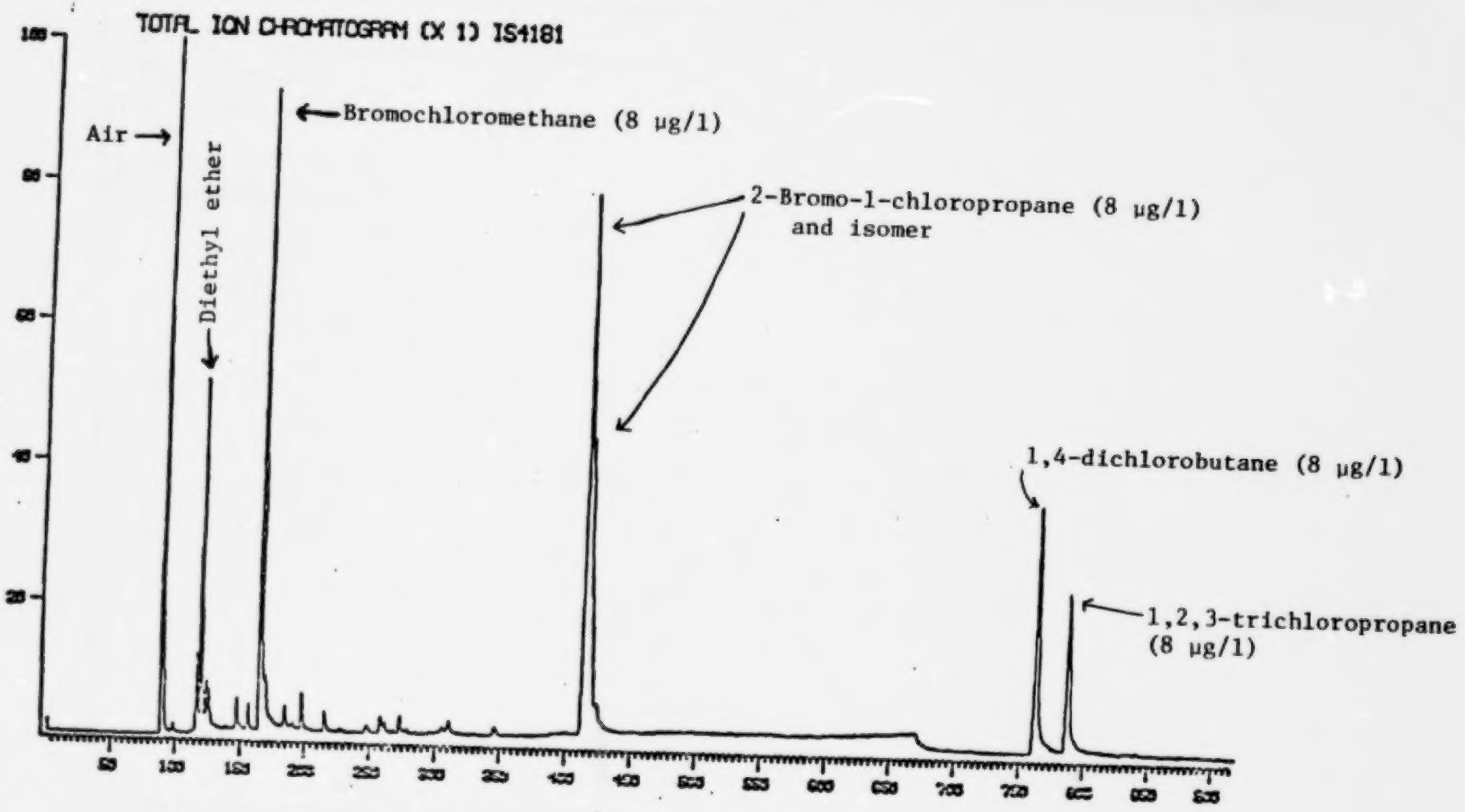


Figure 17. Total ion chromatogram obtained from water spiked with internal standards

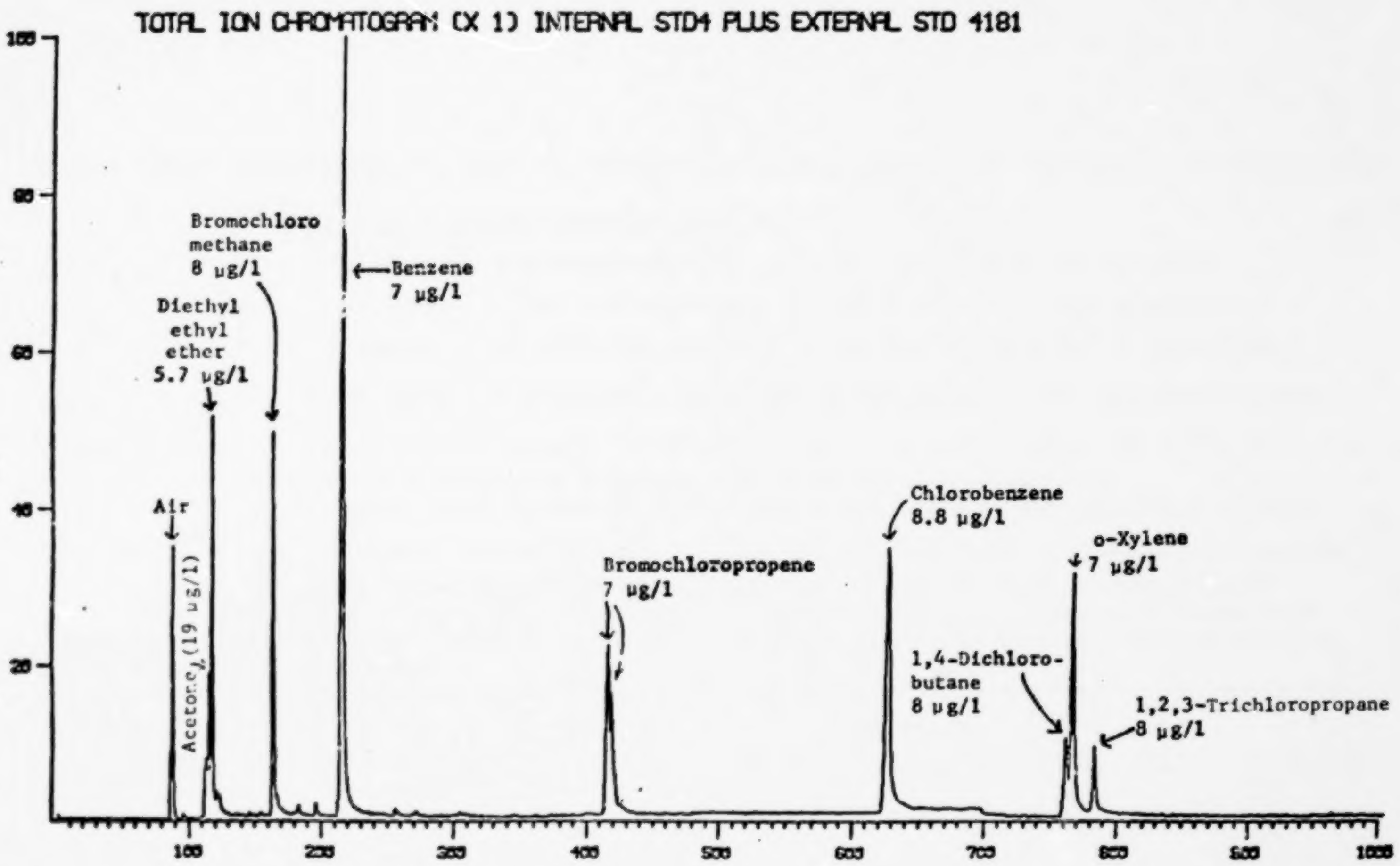


Figure 18. Total ion chromatogram obtained from water spiked with internal standards and external standards

TABLE 7. PRIORITY CRITERIA FOR GC-MS ANALYSIS

Priority	Criteria
0	A zero priority rating is given to any fraction which contains no compounds above a concentration of 4 μg/l or contains compounds 4 μg/l that have been tentatively identified by retention index or GC patterns in context with historical data.
+	A "+" priority rating is given to fractions on the basis of the following criteria. Compounds greater than 4 μg/l but not sufficient for ++ priority.
++	A "++" priority rating is given to fractions on the basis of the following criteria. • 10 or more neutral compounds with conc > 10 μg/l not previously identified • 4 or more acidic compounds with conc > 10 μg/l not previously identified • 2 or more basic compounds with conc > 10 μg/l not previously identified • Conc. of any given compounds $\geq$100 μg/l.

RESULTS AND DISCUSSION

The procedures used to tentatively identify each organic compound, while specific for individual compounds, employed these general operations. First, the GC/MS/COMP analysis of each sample generated many individual mass spectra and total ion chromatograms (TIC). Inspection of each TIC resulted in the selection of a mass spectrum number and a background subtract spectrum number for each "peak" likely to produce a good mass spectrum. Second, a computerized Biemann mass spectral matching system (NIH-EPA data base, ≈25,000 spectra) generated a Similarily Index (S.I.=1.000=perfect match) for the spectrum of each semivolatile compound with a concentration greater than 10 μg/l and selected volatile compounds. The S.I. provided a good first guess as to a compound's identity, but it was unreliable in determining the degree of certainty of a compound's identity. Consequently, many of the mass spectra were manually interpreted and compared to reference spectra in published data bases (2,3) before a tentative identification was made.

Samples containing many and/or concentrated components produced "mixed" mass spectra (two or more compounds eluting simultaneously) in the GC/MS analysis. In many instances of coeluting peaks only general compound names could be assigned (alkyl alcohol, subst. benzoic acid, subst. benzene). Individual isomers and/or members of a class of compounds (C_5-alkylbenzenes, fatty acid methyl esters) were rarely identified because time and funds did not permit the required analyses with authentic compounds. In general, the two limiting factors concerning the tentative identification of organic compounds were the "purity" of each sample component mass spectrum and whether or not each compound's spectrum was in accessible data bases.

TENTATIVE IDENTIFICATION OF VOLATILE COMPOUNDS

The analysis of 63 industrial effluents for purgeable organic compounds resulted in tentative identifications of 159 compounds. In general, the compounds were cleanly separated from each other resulting in clean, easily interpretable spectra. A few samples were selected for Biemann spectral matching on the computer, but most of the compounds were tentatively identified using manual interpretation procedures and the aid of published data bases.(2,3)

Table 8 is a comprehensive list of the volatile compounds tentatively identified in the 63 industrial waste-water effluents and their frequency of occurrence. The purgeable organic compounds tentatively identified in each of the 85 samples (63 effluents, 22 intakes) are listed in tables found in Appendix A.

Table 8. Volatile Compounds Tentatively Identified in 63 Industrial Effluents

Compound[(a)]	Frequency of Occurrence at Given Concentration[(b)]			
	*	**	***	Total
Hydrocarbons				
Aliphatic				
Butene	8	2		10
C_5H_{10}	1			1
C_6H_{14}	1			1
C_7H_{14}	3		1	4
C_7H_{16}	2			2
C_8H_{16}	5	1		6
C_9H_{18}	3	1		4
C_9H_{20}	2			2
$C_{10}H_{12}$	1			1
$C_{10}H_{16}$	1	1		2
$C_{10}H_{20}$	1			1
Cyclohexadiene	1			1
Cyclohexane	3			3
C_3-Alkylcyclohexane	3			3
C_4-Alkylcyclohexane	3			3
Cyclohexene	1			1
Cyclooctatetraene			2	2
Cyclopentadiene		1		1
Cyclopentene	1			1
Decane	4			4
Decene	1	1		2
Diisopropylethane	4			4
Dicyclopentadiene	2			2
Dimethylbutane	9			9

Table 8. (Continued)

Compound[(a)]	Frequency of Occurrence at Given Concentration[(b)]			
	*	**	***	Total
Hexane	2	1		3
Heptane	1			1
Methylcyclohexane	1			1
Methylcyclopentane	9	1		10
Methylpentane	12			12
Nonane	4			4
Octane	1			1
Octene		1		1
Pentane		1		1
Pentene	1			1
Propene		1		1
Trimethylpentene	2			2
Tetramethylcyclopropane	2		1	3
Undecane	1			1
Vinylcyclohexene	3			3
Aromatic				
Benzene (a)	23	5	1	29
Biphenyl			1	1
C_2-Alkylbenzene (a, if ethylbenzene)	19	4	2	25
C_3-Alkylbenzene	11	6		17
C_4-Alkylbenzene	8	2	1	11
C_5-Alkylbenzene	2	1	1	4
Divinylbenzene	1			1
Ethylbenzene (a)	2			2
Indene	1			1
Methylstyrene	4	1	1	6
Naphthalene (a)	3	1		4

Table 8. (Continued)

Compound(a)	Frequency of Occurrence at Given Concentration(b)			
	*	**	***	Total
Styrene	1			1
C_2-Alkylstyrene	3		1	4
Toluene (a)	29	7	5	41
o-Xylene	3			3
m-Xylene	2			2
p-Xylene	2			2
Halo-Compounds				
Aliphatic				
Bromodichloromethane (a)	10	4		14
Bromoform (a)	2			2
Carbon tetrachloride (a)	3	3		6
Chlorobutane	1			1
Chlorobutene	2	1		3
Chloroethane (a)	2			2
Chloroform (a)	25	15	2	42
Chloroprene	1	1		2
Chloropropane	1			1
Chloropropene	2			2
Dibromochloromethane	6	2		8
Dibromoethane	1			1
1,1-Dibromoethane	1			1
Dibromomethane			1	1
Dichlorobutane		1		1
2,3-Dichlorobutane	1			1
Dichlorobutene		1		1
Dichlorocyclooctadiene	1			1
Dichloroethane (a)	13	2		15
Dichloroethylene (a)	18	4		22

Table 8. (Continued)

Compound[a]	Frequency of Occurrence at Given Concentration[b]			
	*	**	***	Total
Dichloromethane (a)	24	27	5	56
Dichloromethylenepropane	1			1
Dichloromethylpropane		1		1
Dichloropropane (a)	9	3		12
Dichloropropene	1			1
Ethyl chloride		1		1
Fluorotrichloromethane	1			1
Tetrachloroethene (a)	6			6
1,1,2,2-Tetrachloroethane (a)	4	1		5
Trichloroethane (a)	5			5
1,1,1-Trichloroethane (a)	31	5		36
Trichloroethylene (a)	11	3		14
Trichlorofluoromethane (a)	2	1		3
1,2,2-Trichloropropane	1			1
Trichlorotrifluoroethane	1			1
Aromatic				
Benzotrifluoride	1			1
Chlorobenzene (a)	2	3	1	6
Chloroethylbenzene	1			1
Chlorotoluene	1	1		2
Dichlorobenzene (a)	6	4	1	11
Trichlorobenzene (a)	1			1
Alcohols, Aldehydes and Ketones				
Aliphatic				
Acetone	5	12	10	27
2-Butene-1-ol	1			1
Butyl ketone	2			2

Table 8. (Continued)

Compound[(a)]	Frequency of Occurrence at Given Concentration[(b)] *	**	***	Total
Butyraldehyde	1	1		2
Crotonaldehyde	1			1
Ethylbutyraldehyde	1			1
2-Ethyl-1-hexanol			1	1
Hexanone	1			1
Heptanone	2			2
Isobutyraldehyde			1	1
Isopropyl alcohol	1		2	3
Methylbutyraldehyde	1			1
Methylcyclopentanone	1			1
Methylethyl ketone	9	2		11
Methylheptanone		1		1
Methylisobutyl ketone	3			3
Methylisopropyl ketone	1			1
Methylpentanone	1	1		2
Methylpropenal	1			1
Methyl-t-butyl ketone	1			1
Nonone	1			1
2-Pentanone	1			1
3-Pentanone	2			2
Ethers and Esters				
Aliphatic				
Butyl acetate	1			1
Butyl ether	1			1
Di-sec-butoxyethane	1			1
Diethyl ether	6	2	1	9
Dihydrofuran		1		1
Diisopropyl ether	6	3	1	10
Dimethyl ether			2	2

Table 8. (Continued)

Compound[a]	Frequency of Occurrence at Given Concentration[b]			
	*	**	***	Total
1,4-Dioxane	1			1
2-Ethyl-1,3-dioxolane		1		1
Ethylisopropyl ether	1			1
Furan	1			1
Methyl-1,3-dioxolane		1		1
Methylethyl-1,3-dioxolane		1		1
Tetrahydrofuran	11	1	1	13
Vinyl formate	1			1
Aromatic				
Diphenyl ether			1	1
Sulfur Compounds				
Carbon disulfide	6	2		8
Carbonyl sulfide		1		1
Diethyl disulfide		1		1
Diethyl sulfide	1			1
Dimethyl disulfide	2	1		3
Dimethyldithiahexane		1		1
Dimethyl sulfide	2		1	3
Dimethylthiacyclopentane	1			1
Dithiahexane		1		1
Ethanethiol	1			1
Ethyl mercaptan	1			1
Ethyl-1-methylethyl disulfide	1			1
Methylethyl sulfide		1		1
Methylpropyl sulfide	1			1
Methylthiacyclohexane	1			1
Methylthiacyclopentane	1			1
Methylthiaethylbenzene	1			1

Table 8. (Continued)

Compound[a]	Frequency of Occurrence at Given Concentration[b]			
	*	**	***	Total
3-Methyl-2-thiapentane	1			1
Thiacyclopentane	1			1
Miscellaneous Compounds				
N-N-Dimethylformamide	1			1
Methoxytrimethylsilane		1		1
Oxazole	1			1
Trimethylsilanol			1	1

(a) Priority pollutant.

(b) Compound concentration levels:
* = <10 µg/l
** = 10-100 µg/l
*** = >100 µg/l

TABLE 9. CLASSIFICATION OF IDENTIFIED PURGEABLE COMPOUNDS

Compound Type	Total No. Identified	Total No. of Occurrences	Priority Pollutants No. Identified	Priority Pollutants No. of Occurrences
Hydrocarbons				
Aliphatic	39	115	0	0
Aromatic	17	154	4	101
Halogenated Compounds				
Aliphatic	35	271	15	240
Aromatic	6	22	3	18
Alcohols, Aldehydes & Ketones				
Aliphatic	23	68	0	0
Ethers and Esters				
Aliphatic	15	45	0	0
Aromatic	1	1	0	0
Sulfur Compounds	19	30	0	0
Miscellaneous Compounds	4	4	0	0
TOTAL	159	710	22	359

The effluent samples analyzed for purgeable components ranged in complexity from those as clean as drinking water to some that were quite smelly and containing compounds with concentrations in the mg/l range. The most polluted samples (number and amount of compounds) were from paint companies. Generally, most volatile compounds were found in the 10-100 µg/l range. The 159 compounds are classified in Table 9.

These compounds range in volatility from chloroethane (b.p. = 12.3°C) to trichlorobenzene (b.p. = 213.5°C), which was also identified in the semivolatile fractions. In some cases, such as C_3-alkylbenzenes, many isomers of the same generic compounds were identified but were classified as one compound in Tables 8 and 9.

Twenty-two purgeable priority pollutants were identified and they occurred 359 times, 51% of the total number of occurrences of volatile compounds. Thirteen priority pollutants occurred in more than 10% of the total samples while only methylene chloride, chloroform, toluene and 1,1,1-trichloroethane occurred in more than half the samples.

TENTATIVE IDENTIFICATION OF NEUTRAL COMPOUNDS

The GC/MS analysis of 33 industrial effluents for neutral semivolatile compounds resulted in the tentative identification of 261 compounds listed in Table 10. Generally, the neutral fractions contained more compounds than either the acidic or basic fractions. Concentration levels were usually in the 10-100 µg/l range but numerous compounds were found in greater than 100 µg/l concentrations. In many cases, the large number and/or high concentration of compounds resulted in coeluting peaks. Consequently, the mass spectra were mixtures of two or more compounds. In many of these cases, only general identifications could be made, if at all. Tables found in Appendix A list the neutral semivolatile compounds tentatively identified in each of the 39 priority rated neutral fractions (33 effluents, 6 intakes). The 261 neutral compounds are classified in Table 11.

Hydrocarbons and halocarbons accounted for about 51% of the compounds while 30% were aromatic compounds. Alkylbenzenes, particularly C_2-alkylbenzenes, occurred the most frequently. Eleven priority pollutants were identified and occurred collectively 46 times, 10% of the 474 total occurrences of neutral compounds.

General patterns concerning the type of industry versus compounds in effluents could not be distinguished in this project due to the limited number of samples. However, some interesting compounds were found, such as: N-methyl-N-nitrosomethanaminobenzene, iodochlorocyclohexane, and substituted benzofuranones.

TENTATIVE IDENTIFICATION OF ACIDIC COMPOUNDS

The GC/MS analysis of 26 industrial effluents for acidic semivolatile compounds resulted in the tentative identification of 104 compounds. The compounds listed in Table 12 are names as the parent compound, although methylation with diazomethane meant that certain acidic compounds were actually identified as methyl esters and/or methyl ethers.

Table 10. Neutral compounds tentatively identified in 33 industrial effluents

COMPOUND[a]	SAMPLE NO.[b]	Frequency of Occurrence at Given Concentration[c]			
		*	**	***	TOTAL
Straight or Branched Chain Compounds					
Hydrocarbons					
Heptane	31E			1	1
Alkane C $\geq$ 8	31E	1	1		2
Alkane C $\geq$ 9	31E	2	1	1	4
Decane	54E	2	3		5
Branched Hydrocarbon	1E		1		1
Undecane	54E	4	1		5
Alkane C $\geq$ 11	12E	1	1		2
Dodecane	26E	1	1		2
Alkane C $\geq$ 12	12E	1		1	2
Tridecane	54E	1	1		2
Alkane C $\geq$ 13	54E	2	1	1	4
Tetradecane	29E	1		2	3
Alkane C $\geq$ 14	29E	2	1	1	4
Pentadecane	29E	1	2	1	4
Alkane C $\geq$ 15	54E		1		1
Hexadecane	54E	1	1	2	4
Alkane C $\geq$ 16	25E		2	1	3
Heptadecane	29E	3	2	1	6
Alkane C $\geq$ 17	54E	2		1	3
Octadecane	25E		1	1	2
Alkane C $\geq$ 18	29E		2		2
Nonadecane	25E	1	3		4
Alkane C $\geq$ 19	26E		2		2
Eicosane	4E	1	2		3
Heneicosane	26E	1	3		4
Alkane C $\geq$ 21	29E	1	1		2
Docosane	26E		1		1
Tricosane	26E		1		1
Branched Hydrocarbon C $\geq$ 23	1E	1			1
Tetracosane	1E		1		1

Table 10. (Continued)

COMPOUND[a]	SAMPLE NO.[b]	Frequency of Occurrence at Given Concentration[c]			
		*	**	***	TOTAL
Alkane C ≥ 24	58E		1		1
Pentacosane	40E		2		2
Alkane C ≥ 25	26E		1		1
Hexacosane	26E		1		1
Heptacosane	26E		2		2
Octacosane	26E		1		1
Nonacosane	26E		1		1
Nonene	33E		1		1
Methyloctene	29E		1		1
Decene	29E			1	1
Methylnonene	33E		1		1
Alkene C ≥ 11	25E	1			1
Dodecene	29E			1	1
Alkene C ≥ 12	31E	1	1		2
Alkene C ≥ 13	26E			1	1
Tetradecene	29E			2	2
1-Propene-2-methyl trimer	34E		1		1
Alkene C ≥ 15	29E		1		1
Hexadecene	29E			1	1
Alkene C ≥ 17	29E			1	1
Octadecene	29E		1		1
Alkene C ≥ 19	29E		1		1
Eicosene	29E		1		1
1-Propene-2-methyl tetramer	34E		1		1
Alkene C ≥ 20	29E		1		1
Alkene C ≥ 22	29E		1		1
Alkene C ≥ 23	29E		1		1
Alkene C ≥ 27	29E		1		1
Alkene C ≥ 29	29E		1		1
Dimethyldecene	29E			1	1

Table 10. (Continued)

COMPOUND[a]	SAMPLE NO.[b]	Frequency of Occurrence at Given Concentration[c]			
		*	**	***	TOTAL
Halocarbons					
1,3-Butadiene,2-chloro-dimer	34E			1	1
$C_4H_6Cl_2$	45E			1	1
Chloroalkene	45E			1	1
Chlorohydrocarbon	58E	1			1
Dichlorobutene	45E		1		1
Dichloropropene	35E		1		1
Halo-alkane	4E	1			1
Halo-alkene	21E		1		1
Iodoheptane	49E			1	1
Tetrachloroethane	60E	1			1
Alcohols					
Alkyl alcohol	31E		5		5
Alkyl alcohol C $\geq$ 8	31E		1		1
Alkyl alcohol C $\geq$ 9	22E		3		3
Alkyl alcohol C $\geq$ 11	25E	1	1		2
Alkyl alcohol C $\geq$ 12	22E	1	2	1	4
Dimethylpentanol	35E		1	1	2
Docosanol	29E		1		1
Eicosanol	8E	1			1
Heptadecanol	35E		1		1
Hexenol	21E			1	1
Methylheptanol	31E			1	1
Octanol	29E		1		1
Propylheptanol	29E			1	1

Table 10. (Continued)

COMPOUND[a]	SAMPLE NO.[b]	Frequency of Occurrence at Given Concentration[c]			
		*	**	***	TOTAL
Ethers					
Alkyl ether	33E		2		2
Alkenyl ether	33E		1		1
2-Butoxyethanol	30E	1	4		5
n-Butyl ether	7E	1			1
Ethanol,2-(1-(2-butyoxy ethoxy)	7E	1			1
Ethanol,1-(2-butoxy ethoxy)	45E			1	1
Hexexy butanol	15E	1			1
2-Propanol,1-(2-methoxy-1-1 methyl ethoxy)	50E		1		1
2-Propanol,1-(2-methoxy-1-methyl ethoxy)-isomer	50E		1		1
Ketones					
Alkyl diketone	7E	1			1
Alkyl ketone C $\geq$ 7	22E	1	1		2
Alkyl ketone C $\geq$ 10	34E		1		1
Alkyl ketone C $\geq$ 11	22E		1		1
Alkyl ketone C $\geq$ 27	22E		1		1
Dimethylpentanone	28E		2		2
Heptanone	6E	2			2
Isophorone	7E	2			2
Methyl hexanone	22E			1	1
Methyl pentanone	45E	1			1
4-Octanone	8E	1			1
Aldehydes					
Aldehyde $C_8H_{16}O$	35E		1		1
Methylpentanal	21E	1			1

Table 10. (Continued)

COMPOUND[a]	SAMPLE NO.[b]	Frequency of Occurrence at Given Concentration[c]			
		*	**	***	TOTAL
Esters					
Acetic acid C $\geq$ 8 ester	34E		1		1
Acetic acid C $\geq$ 9 ester	34E		1		1
Butyl acetate	26E			1	1
Propanoic acid-2-methyl propyl	28E		1		1
Cyclic Nonaromatic Compounds					
Hydrocarbons					
Alkylcyclohexane	9E	2			2
Alkylcyclohexene	49E		1		1
1,1'-Bicyclohexyl, ethyl	49E		1		1
Methylcyclohexane	49E	1		1	2
Halocarbons					
Bromochlorocyclohexane	21E	2	3	2	7
Chlorocyclohexane	49E	1			1
Chlorocyclohexene	15E	1	4		5
1-Chloro-5-(1-chloroethenyl) cyclohexene	34E		1		1
Dibromocyclohexane	5E	4			4
Dibromocyclohexene	15E	1			1
Dichlorocyclohexane	15E		1	3	4
Halo-cyclohexane	77E	1			1
Iodochlorlcyclohexane	49E			1	1
Subst. iodocyclohexane	49E	1			1
Alcohols					
Bromocyclohexanol	15E	2	4	1	7
C_4-Alkylcyclohexanol	22E		2		2

Table 10. (Continued)

COMPOUND[a]	SAMPLE NO.[b]	Frequency of Occurrence at Given Concentration[c]			
		*	**	***	TOTAL
Chlorocyclohexanol	15E	2	4	2	8
Cyclohexenol	15E		2		2
Methylcyclohexanol	22E		1		1
Ethers					
Bromomethoxycyclohexane	15E		2		2
Oxybisyclo[4,1,0]heptane	15E		1		1
Ketones					
Alkylcyclohexanone	33E		1		1
C_3-Cyclohexadienone	33E		1		1
C_3-Cyclohexenone	33E		1		1
Chlorocyclohexanone	9E	1			1
Methylcyclohexanone	22E		1		1
Methylcyclohexenone	35E	1	1		2
Esters					
Subst. cyclohexene carboxylic acid methyl ester	40		1		1
Aromatic Compounds					
Hydrocarbons					
Alkyl benzene	7E	3			3
Alkyl indene	33E		1		1
Alkyl naphthalene	12E	2	1		3
Alkyl tetrahydronaphthalene	45E			1	1
1,1'-Biphenyl	14E	1	3	3	7
C_3-Alkylbenzene	26E	1	6	2	9
C_4-Alkylbenzene	26E	1	3	1	5
C_5-Alkylbenzene	25E	1	1	2	4
C_6-Alkylbenzene	35E		1		1

Table 10. (Continued)

COMPOUND[a]	SAMPLE NO.[b]	Frequency of Occurrence at Given Concentration[c]			
		*	**	***	TOTAL
C_2-1,1'-Biphenyl	25E		1		1
C_2-Alkyldihydroindene	4E	1			1
C_2-Alkyldihydronaphthalene	12E	1			1
C_2-Alkylstyrene	35E		2		2
C_3-Alkynylbenzene	35E		1		1
C_3-Alkylstyrene	25E		2		2
C_2-Phenanthrene	1E	1			1
C_3-Phenanthrene	1E	1			1
Dihydrodimethylindene	32E		1		1
Dihydronaphthalene	60E		3		3
Dimethylnaphthalene	54E			1	1
Ethylbenzene (a)	26E	2	6	2	10
Ethylstyrene	30E	1	1		2
Indene	32E		1		1
1H-Indene-1-ethyl-2,3-dihydro	25E		1		1
Methyl-1,1'-biphenyl	25E	1			1
Methylindene	32E		2		2
Methylnaphthalene	26E		4	1	5
Methyl phenanthrene	1E	1			1
Methylstyrene	26E		2		2
Methyltetrahydronaphthalene	35E		1		1
Naphthalene(a)	26E	3	3	1	7
Styrene	31E			1	1
Subst.-alkylbenzene	32E		1		1
Subst.-benzene	31E		1		1
Subst.-benzene isomer	31E			1	1
Subst. styrene	31E		1		1
Tetrahydrodimethylnaphthalene	32E		1		1
1,2,3,4-Tetrahydronaphthalene	7E		1		1
Toluene (a)	14E	2	6		8
Xylene	28E	1	5	2	8

Table 10. (Continued)

COMPOUND[a]	SAMPLE NO.[b]	Frequency of Occurrence at Given Concentration[c]			
		*	**	***	TOTAL
Halocarbons					
Bromonaphthalene	49E	1			1
Chlorobenzene(a)	49E	2	2		4
Chloromethylbenzene	60E	1			1
1,2-Dichlorobenzene(a)	7E		2		2
1,3-Dichlorobenzene(a)	7E	1			1
1,4-Dichlorobenzene(a)	7E	1			1
Dichloromethylbenzene	60E		1		1
Tetrachlorobenzene	60E	1			1
1,2,4-Trichlorobenzene (a)	60E		1		1
Tribromoethylbenzene		1			1
Alcohols					
Tetrahydromethylnaphthalenol	12E	1			1
Ethylbenzenemethanol	6E	1			1
1-Methyl-1-phenylethanol	28E		1	2	3
1,4-Methanonaphthalen-9-ol,1,4-dihydro	14E	1			1
1-Phenylpropanol	15E	1	1		2
Tetrahydromethylnaphthalenol	12E	1			1
Ethers					
Benzene,1,1'-Oxybis(4-methyl)	45E			1	1
1,1'-Biphenyl,2-phenoxy	7E	1			1
Diphenyl ether	28E	2		3	5
Methoxy-C_3-benzene	29E			1	1

Table 10. (Continued)

COMPOUND[a]	SAMPLE NO.[b]	Frequency of Occurrence at Given Concentration[c]			
		*	**	***	TOTAL
Ketones					
Acetophenone	45E	2	1		3
Alkylaromatic ketone	8E	1			1
Alkyl-naphthalenone	4E	1			1
Dihydroindenone	35E	1	2	1	4
Dihydro-1H-Inden-1-one	35E		1		1
o-Methoxypropylphenone	45E		1		1
1-Phenylpropanone	15E	1	1	1	3
2-Propanone,4-methyl-4-phenyl	7E	1			1
1,2,3,4-Tetrahydronaphthalen-1-one	7E		1		1
Aldehydes					
Benzaldehyde	9E	1		1	2
Ethanone,1-[4-(1-methylethyl) phenyl	25E		1		1
Ethanone,1-(2,4-dimethylphenyl)	4E	1			1
Esters					
Benzoic acid,2-propenyl ester	45E		1		1
Benzene methanol, methoxy acetate	58E		1		1
Bis(2-ethylhexyl) phthalate (a)	50E	2	1		3
Butylbenzyl phthalate(a)	26E	1	2		3
Di-2-propenyl phthalate	45E			1	1
Dibutyl phthalate (a)	14E	5	1		6
Diethyl phthalate	40E	1	1		2
Phthalate	45E	5			5
Sulfur Compounds					
Benzene-1,1'-sulfonyl bis-	63E	1			1
Benzene,1,1'-sulfonyl bis[4-chloro-]	63E			1	1

Table 10. (Continued)

COMPOUND[a]	SAMPLE NO.[b]	Frequency of Occurrence at Given Concentration[c]			
		*	**	***	TOTAL
N-Dimethylbenzene sulfonamide	14E	1			1
2,3-Dithiahexane	25E		1		1
3,4-Dithiahexane	25E		1		1
Methyl,4-chlorophenyl sulfone	63E	1			1
Methyldithiahexane	25E		1		1
Nonanethiol	33E		1		1
Nitrogen Compounds					
Benzene methanamino,N-methyl, N-nitroso	50E			1	1
N,N-Dimethylacetamide	14E	1			1
Nitroaniline	50E		1		1
Nitrobenzene	51E			1	1
Nitrocyclohexene	51E		1		1
Phosphorus Compounds					
Phosphordithioic acid,0,0-dimethyl-S-ethyl ester	45E		1		1
Subst. Phosphate	7E	1			1
Trialkylphenyl phosphate	7E		1		1
Tributyl phosphate	5E	1	1		2
Tricresyl phosphate	7E		1		1
Triphenylester, phosphoric acid	7E		1		1
Trixylyl phosphate	7E		1		1
Trioctyl phosphate	1E	1			1
Silicon Compounds					
Silicone		2	1		3
Hetrocyclic Compounds					
Alkylphenol C $\geq$ 15	22E		1		1

Table 10. (Continued)

COMPOUND[a]	SAMPLE NO.[b]	Frequency of Occurrence at Given Concentration[c]			
		*	**	***	TOTAL
3(2H)Benzofuranone, Dimethyl	45E		1		1
3(2H)Benzofuranone, Methyl	25E		3		3
1,2,3-Benzothiadiazole	12E			1	1
Dibenzofuran	14E	1			1
Dihydromethylfuranone	60E	1			1
Dimethylbenzofuran	35E		1		1
1,3-Dioxolane,2-(chloromethyl)	50E		1		1
Methylbenzothiazole	60E	1			1
2-Propenal-3(2-furanyl)	45E		1		1
1,2-Benzisothiazol,3-ethoxy,1,1-dioxide	45E		1		1
Tetrahydrothiaphene,1,1-dioxide	32E			1	1
Subst. benzofuranone	45E			1	1
Miscellaneous Compounds					
Alkylphenol C $\geq$ 15	22E		1		1
Alkylphenol C $\geq$ 16	22E		1		1
2,4-Bis(1-methylethyl) phenol	7E		1		1
2,4-Bis(1-methylbutyl)phenol	50E		1		1
2,4-Bis(1-methylethyl) phenol	7E		1		1
C_4-Alkylphenol	45E			1	1
C_4-N,N-Subst. aniline	29E		1		1
Chloroalkyl subst. phenol	50E		1		1
Subst. phenol	7E	1			1

(a) Priority pollutant

(b) Representative sample in which compound was identified (see Appendix A)

(c) Compound Concentration Levels:
* = <10 μg/l
** = 10-100 μg/l
*** = >100 μg/l

Table 11. Classification of Compounds Identified in Neutral Fractions

Compound Type	Total No. Identified	Total No. of Occurrences	Priority Pollutants No. Identified	Priority Pollutants No. of Occurrences
Straight or Branched Chain Compounds				
Hydrocarbons	60	115	0	0
Halogenated compounds	10	10	0	0
Alcohols	13	24	0	0
Ethers	9	14	0	0
Ketones	11	15	0	0
Aldehydes	2	2	0	0
Esters	4	4	0	0
Cyclic Non-aromatic Compounds				
Hydrocarbons	4	6	0	0
Halogenated compounds	10	26	0	0
Alcohols	5	20	0	0
Ethers	2	3	0	0
Ketones	6	7	0	0
Esters	1	1	0	0
Aromatic Compounds				
Hydrocarbons	40	105	3	25
Halocarbons	10	14	5	9
Alcohols	6	9	0	0
Ethers	4	8	0	0
Ketones	9	16	0	0
Aldehydes	3	4	0	0
Esters	8	22	3	12
Sulfur Compounds	8	8	0	0
Nitrogen Compounds	5	5	0	0
Phosphorous Compounds	8	9	0	0
Silicon Compounds	1	3	0	0
Heterocyclic Compounds	13	15	0	0
Miscellaneous Compounds	9	9	0	0
TOTAL	261	474	11	46

Table 12. Acidic Compounds Tentatively Identified in 26 Industrial Effluents

COMPOUND[a]	SAMPLE NO.[b]	Frequency of Occurrence at Given Concentration[c]			
		*	**	***	TOTAL
Aliphatic Acids					
Alkenoic Acid C $\geq$ 18	9E	1			1
Alkenoic acid (branched)			1		1
Acetoxyhexanoic acid	35E		1		1
Benzeneacetic acid	53E		3		3
Benzenepropanoic acid	53E		1		1
C_3-Alkylphenylpropanoic acid	35E		1		1
Dimethylbutanoic acid	35E	1			1
Dimethylphenylpropanoic acid	35E		1		1
Fatty acids					
3-Methylpentanoic acid	35E		2		2
Hexanoic acid	62E		1		1
C $\geq$ 6	31E	1	7	1	9
Heptanoic acid	26E		1		1
C $\geq$ 7	31E	3	3	1	7
Octanoic acid	26E		3		3
C $\geq$ 8	31E	2	1	2	5
Nonanoic acid	26E		1		1
C $\geq$ 9	31E	1	1	1	3
Decanoic acid	26E		1		1
C $\geq$ 10	31E	2	2		4
Dodecanoic acid	26E	3	4		7
C $\geq$ 11	29E		1		1
C $\geq$ 12	43E	2			2
C $\geq$ 13	62E	1			1
Tetradecanoic acid	26E	6	5		11
C $\geq$ 14	35E	2	3		5
Pentadecanoic acid	53E	2	1		3

Table 12. (Continued)

COMPOUND[a]	SAMPLE NO.[b]	Frequency of Occurrence at Given Concentration[c] *	**	***	TOTAL
C ≥ 15	18E	5	3		8
Hexadecanoic acid	29E		7	2	9
C ≥ 16	18E	3	4		7
Heptadecanoic acid	56E	1			1
C ≥ 17	56E	4	3		7
Octadecanoic acid	26E	5	3		8
C ≥ 18	31E	5	5	1	1
C ≥ 19	53E	1			1
Eicosanoic acid	9E	1			1
C ≥ 20	40E	1	2		3
C ≥ 21	40E	1	1		2
C ≥ 22	40E	1	1		2
C ≥ 23	40E		1		1
C ≥ 24	40E		1		1
Methylcyclohexene-1-carboxylic acid	22E		2		2
Methylphenylpropanoic acid	35E		1		1
Octadecadienoic acid	26E	1	2	1	4
Octadecenoic acid	26E	2	2	2	6
Subst. cyclohexane acid	2E	1			1
Aromatic Acids					
Alkylbenzoic acid	35E		2		2
Benzenedicarboxylic acid	50E		1		1
Benzoic acid	28E	2	8	1	11
C_5-Alkyloctahydrophenanthrene carboxylic acid	58E		2		2
Dimethylbenzoic acid	35E		1		1
Ethenylbenzoic acid	35E		1		1
Methylbenzoic acid	26E		3		3
Octahydro-1,4-dimethyl-1-(methylethyl)phenanthrene carboxylic acid	52E		1		1

Table 12. (Continued)

COMPOUND[a]	SAMPLE NO.[b]	Frequency of Occurrence at Given Concentration[c]			
		*	**	***	TOTAL
Octahydrodimethylphenanthrene carboxylic acid	22E		1		1
Subst. phenanthrene carboxylic acid	31E		3		3
Subst. benzoic acid	12E	1	1		2
Trimethylbenzoic acid	26E		2		2
Haloaliphatic Acids					
Chloro-fatty acid	9E	1			1
Halo-acid	9E	1			1
Haloaromatic Acids					
Chlorobenzoic acid	60E		2		2
Chloroalkylbenzoic acid	12E	1			1
Dichlorobenzoic acid	60E	2			2
Alkylphenols					
Alkylphenol	34E		1		1
Benzene[(dihydroxy)methyl]	58E	1			1
Benzene,1-hydroxy-2-[(4-hydroxyphenyl)]	58E	1			1
C_2-Alkylphenol	44E			1	1
C_3-Alkylphenol	44E		1		1
C_4-Alkylphenol	44E	1	2		3
C_4-Alkenylphenol	44E		1		1
Dimethylphenol(a)	43E		4		4
Isomer of phenol 2-[(4-hydroxyphenyl)methyl]	58E	1			1

Table 12. (Continued)

COMPOUND[a]	SAMPLE NO.[b]	Frequency of Occurrence at Given Concentration[c]			
		*	**	***	TOTAL
Methylallylphenol	44E		1		1
Methylphenol	29E	1	5	3	9
Nonylphenol	22E		1		1
Phenol(a)	60E		5	7	12
Phenol,2,6-[4-(hydroxyphenyl) dimethyl]	52E		2		2
Phenol,2-[4-(hydroxyphenyl)methyl]	52E		1	1	2
Halophenols					
Bromomethylphenol	53E		3		3
Bromophenol	52E	1	4		5
Chloroalkylphenol	58E	1			1
Chlorobromosubst.-phenol	58E	1			1
Chlorophenol(a)	52E		3	4	7
Chloromethylphenol(a)	57E	1	2		3
Dichlorophenol(a)	58E		3		3
Trichlorophenol(a)	50E	1	2		3
Benzenesulfonic Acid Derivatives					
Benzenesulfonic acid-4-hydrocyhydrazide	34E		1		1
Benzenesulfoniamide,N,4-dimethyl	52E	2	2		4
p-Toluenesulfonamide	9E		3		3
Subst.-benzenesulfonic acid	34E		1		1
Heterocyclic Compounds					
Benzothiadiazole	12E	1			1
Methoxy-1,2-benzothiazole	60E		1		1
Methoxythiiobenzothiazole	60E		1		1
Subst.-benzisothiazole	60E	1			1

Table 12. (Continued)

COMPOUND[a]	SAMPLE NO.[b]	Frequency of Occurrence at Given Concentration[c] *	**	***	TOTAL
Miscellaneous Compounds					
Allylthiopropanoic acid	35E	1			1
Dihydroxybenzaldehyde	58E	1			1
Dimethylhydroxybenaldehyde	18E		1		1
Hydroxybenzoic acid	32E	2			2
Hydroxybenzeneacetic acid	50E	1			1
Hydroxytrimethylbenzoic acid	50E	1			1
Hydroxymethylbenzoic acid	35E		1		1
Indolinecarboraldehyde, hydroxymethyl	18E		1		1
Oxiraneoctanoic acid,2-octyl	9E		1		1
Octadecanoic acid,9,10-dihydroxy	9E		1		1
Thienopyridine	60E		1		1

(a) Priority Pollutant

(b) Representative sample in which compound was identified (see Appendix A)

(c) Compound Concentration Levels:
* = <10 μg/l
** = 10-100 μg/l
*** = >100 μg/l

TABLE 13. CLASSIFICATION OF COMPOUNDS IDENTIFIED IN ACID FRACTIONS

Compound Type	Total No. Identified	Total No. of Occurrences	Priority Pollutants No. Identified	Priority Pollutants No. of Occurrences
Aliphatic acids	45	143	0	0
Aromatic acids	12	30	0	0
Halo-aliphatic acids	2	2	0	0
Halo-aromatic acids	3	5	0	0
Alkylphenols	15	41	2	16
Halophenols	8	26	4	16
Benzenesulfonic acid derivatives	4	9	0	0
Heterocyclic compounds	4	4	0	0
Miscellaneous compounds	11	12	0	0
TOTAL	104	272	6	32

Because mass spectra of many of these methylated compounds were not included in accessible data bases the number of tentative identifications in the acidic fractions was limited. Tables in Appendix A list the acidic semivolatile compounds tentatively identified in each of the 29 priority rated acidic fractions (26 effluents, 3 intakes).

The acidic fractions of the 26 effluent samples analyzed were generally less complex than the neutral fractions but contained more components than the basic fractions. Most acidic compounds were found with concentrations of 10-100 μg/l. No particular type of company had effluents which could be distinguished from one another on the basis of their acidic compound content (concentration and number of compounds). The 104 acidic compounds are classified in Table 13.

Not surprisingly, aliphatic acids were the most numerous compounds followed by alkylphenols and aromatic acids. Six priority pollutants were identified - phenol (12 times), chlorophenol (7 times), dichlorophenol (3 times), trichlorophenol (3 times), dimethylphenol (4 times) and chloromethylphenol (3 times). Fifty-six compounds occurred only once, while phenol and benzoic acid occurred 12 and 11 times respectively. The acidic compounds occurred a total of 272 times while priority pollutants accounted for only 32 occurrences, about 12% of the total number of occurrences.

TENTATIVE IDENTIFICATION OF BASIC COMPOUNDS

The analysis of 21 industrial effluents for basic semivolatile compounds resulted in the tentative identification of 49 compounds listed in Table 14. Tables found in Appendix A list the basic compounds tentatively identified in each of the 21 effluent samples.

Generally, the basic compounds found in the effluent samples were present in smaller numbers and lower concentration (<10 μg/l) compared to the neutral and acidic compounds. Steel companies, as a group, had effluents with the highest number of basic compounds, and in some cases, the basic compounds were the most concentrated components in the sample. It should be noted that all the basic compounds present in the effluent extracts probably did not elute from the SE-30 capillary column. This result was expected--future analyses should use a more suitable column for basic components. The 49 basic compounds are classified in Table 15.

The basic compounds occurred a total of 70 times while no priority pollutants were identified. Methyl pyridine occurred most frequently (8 times) while 39 of the 49 compounds occurred only once. The heterocyclic compounds would appear to be the most interesting group of compounds both in biological activity and environmental significance.

Table 14. Basic Compounds Tentatively Identified in 21 Industrial Effluents

COMPOUND[a]	SAMPLE NO.[b]	Frequency of Occurrence at Given Concentration[c]			
		*	**	***	TOTAL
Aliphatic Amines					
Alkyl amine	22E	1	1		2
Cyclohexyl amine	52E			1	1
Hexamethylenetetramine	56E		1		1
N-Butyl-1-butamine	62E			1	1
N-Butyl,N-methyl-1-butamine	62E	1	1		2
N-Phenylmethyleneheptamine	22E	1			1
Aromatic Amines					
Diethylaniline	29E		1		1
Dimethylaniline	30E	2	3		5
Methylaniline	50E	1	1	1	3
N-Ethyl-o-toluidine	29E	1			1
N,N-Diethylaniline	54E	1			1
Pentamethylaminobenzene	45E		1		1
Heterocyclic Compounds					
Alkylaziridine ($C_8H_{17}N$)	22E			1	1
Benzo[c]methylcinnoline	18E		1		1
C_3-Alkylpyridine	54E	2			2
C_4-Alkylpiperidine	45E		1		1
C_4-Alkylpyridine	33E	2	1		3
C_5-Alkylpyridine	33E		1		1
C_5-Alkylquinoline	34E	1			1

Table 14. (Continued)

COMPOUND[a]	SAMPLE NO.[b]	Frequency of Occurrence at Given Concentration[c]			
		*	**	***	TOTAL
C_3-Benzimidazole	18E		1		1
Dimethylbenzimidazole	18E		1		1
2,6-Dimethyl-4-ethylpyridine	33E		1		1
Dimethylnaphthyridine	18E	1			1
Dimethylquinoline	32E	1			1
Imidazolidine,C_2-alkylphenyl	49E	1			1
Imidazolidine,C_3-alkylphenyl	49E	1			1
Isoquinoline	18E		1		1
Methylbenzimidazole	18E		1		1
3-Methylcinnoline	18E		2		2
Methylisoquinoline	18E		1		1
Methylnaphthyridine	18E		1		1
Methylpyridine	18E		5	3	8
1,6-Naphthrydine	18E		1		1
Phenanthroline	18E		1		1
Phenothiazine	34E		1		1
Pyridine,3-(1-Methyl-2-pyrrolidinyl)	54E	1			1
Pyrrolo(2,3,8-pyridine, dimethyl	18E		1		1
Quinoline	53E	1	1		2
Trimethylpiperidine	45E		1		1
Trimethylpyridine (2 isomers)	33E			1	1
Miscellaneous Compounds					
Cyanopyridine	22E		1		1
2-Diethylaminoethanol	52E			1	1
5-Hexen-3yn-2-one,6-(1-piperidinyl)	52E		1		1
Hydroxymethylimidazole	52E			1	1

Table 14. (Continued)

COMPOUND[a]	SAMPLE NO.[b]	Frequency of Occurrence at Given Concentration[c]			
		*	**	***	TOTAL
2-Methoxyaniline	50E			1	1
Methoxyaniline	45E		2		2
3-Methyl-5-ethoxypyrazole	50E		1		1
2-Propen-1-amine,N,N-di-2-propenyl	34E		1		1
1,3,5-Triazine-2,4-diamine,6-(3-methyl-phenyl	34E	1			1

(a) Priority Pollutant

(b) Representative sample in which compound was identified (see Appendix A)

(c) Compound concentration levels:

* = <10 μg/l
** = 10-100 μg/l
*** = >100 μg/l

TABLE 15. CLASSIFICATION OF COMPOUNDS IDENTIFIED IN BASIC FRACTIONS

Compound Type	Total No. Identified	Total No. of Occurrences	Priority Pollutants No. Identified	Priority Pollutants No. of Occurrences
Aliphatic amines	6	8	0	0
Aromatic amines	6	12	0	0
Heterocyclic compounds	28	40	0	0
Miscellaneous compounds	9	10	0	0
TOTAL	49	70	0	0

SUMMARY OF IDENTIFIED COMPOUNDS IN INDUSTRIAL EFFLUENT SURVEY

During the course of this industrial effluent survey many different types of data have been generated. Correlation of these different data types can be done in a number of ways depending upon one's perspective and interests. Table 16 correlates the number of identified compounds with various other parameters. This representation may be useful in determinating the environmental significance of compounds found in industrial effluents.

TABLE 16. SUMMARY OF IDENTIFIED COMPOUNDS IN INDUSTRIAL EFFLUENT SURVEY

Sample Type	No. of Effluents Analyzed	No. of Compounds Identified	Total No. of Occurrences	No. Found in Only One Effluent	Priority Pollutants	
					No. Identified	Total No. of Occurrences
Purged Effluent	63	159	710	85	22	359
Extract-neutral fraction	33	261	474	176	11	46
Extract-acid fraction	26	104	272	56	6	32
Extract-basic fraction	21	49	70	39	0	0
TOTAL		573[(a)]	1526	356	39[(b)]	437

(a) Because some purged compounds were also present in extracts, less than 573 different compounds were identified.

(b) Toluene, ethylbenzene, chlorobenzene, dichlorobenzene trichlorobenzene, and naphthalene were found in both purgeable and neutral fractions. A total of 33 different priority pollutants were identifed in this survey.

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APPENDIX A

SAMPLE DATA TABLES

TABLE A-1. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 1VE

GC Peak No.	Relative Retention Time	Amount µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.16		Air	44(100)
2	0.18	<1	Butane or Methylpropane	43(100)58(50)
3	0.20	1-10	Acetone	43(100)58(60)
4	0.20	<1	Dichloroethylene	61(100)96(80)98(55)
5	0.21	1-10	Dichloromethane	49(100)51(33)84(85)86(55)
6	0.21	<1	Carbon Disulfide	76(100)78(4)
7	0.24	10-100	Butyraldehyde	44(100)43(85)72(55)41(52)57(30)
8	0.26	1-10	Chloroform	83(100)85(66)
9	0.28	<1	Tetrahydrofuran	42(100)41(50)72(30)71(30)43(20)
10	0.29	<1	Methylcyclopentane	56(100)41(60)69(40)55(30)42(20)
11	0.30	1-10	1,1,1-Trichloroethane	97(100)99(65)61(55)63(20)117(10)119(11)121(5)
12	0.32	<1	Benzene	78(100)77,50-52(20)
13	0.57	<1	Toluene	91(100)92(60)
14	0.91	<1	C_2 Alkyl Benzene	91(100)106(40)
15	0.97	<1	C_2 Alkyl Benzene	91(100)106(65)
16	1.00	~(8)	I.S.	75(100)77(33)110(30)61(25)
17	1.00	<1	Methylethyl Cyclohexane	55(100)97(55)41(30)126(8)
18	1.01	<1	Methylethyl Cyclohexane	55(100)97(80)41(70)126(15)
19	1.05	<1	Methylethyl Cyclohexane	55(100)97(95)41(35)126(12)
20	1.06	<1	Methylethyl Cyclohexane	55(100)97(90)96(40)81(30)126(18)
21	1.09	<1	C_4 Cyclohexane	55(100)82(80)83(70)41(50)67(65)126(10)
22	1.10	<1	Methylethyl Cyclohexane	97(100)55(98)41(30)69(25)126(8)
23	1.11	<1	C_4 Cyclohexane	83(100)55(98)82(65)41(40)
24	1.14	<1	Diethyl Cyclohexane	69(100)111(70)55(50)41(38)
25	1.15	<1	M 126 Hydrocarbon	57(100)71(70)43(65)
26	1.17	<1	4-n-Propylheptane	57(100)43(68)98(15)
27	1.18	<1	Unknown Hydrocarbon	69(100)70(70)55(65)125(60)

TABLE A-2. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 1E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	KI x 10^3
1	929	**	Branched Hydrocarbon C > 9	43 (100) 57 (88) 41 (76) 85 (34) 71 (25) 56 (25) 128 (5)	Nonane	546
2	1010	**	Branched Hydrocarbon C > 10	43 (100) 57 (90) 41 (70) 71 (35) 85 (25) 142 (5)	Decane	376
3	1103	**	Undecane		Undecane	383
4	1202	*	Silicone	267 (100) 73 (30) 268 (29) 251 (18) 269 (18)		
5	1211	*	Branched Hydrocarbon C > 12	43 (100) 57 (99) 41 (79) 71 (52) 85 (32) 170 (3)	Undecane	530
6	1685	**	Hexaethylbenzene	Internal Standard		
7	1706	*	Heptadecane		Heptadecane	377
8	1714	*	Branched Hydrocarbon C > 17		Heptadecane	523
9	1836	*	Methylphenanthrene	192 (100) 191 (62) 189 (31) 193 (22) 165 (18)	2-Methylphenanthrene	303
10	1886	*	?		2-Methyldecanol	378
11	1905	*	Phthalate		1,2-Benzenedicarboxylic Acid Butyl, 2-	476
					Methylpropyl Ester	
12	1978	*	C_2-Phenanthrene	206 (100) 191 (33) 189 (29) 205 (23) 207 (20)	3,6-Dimethylphenanthrene	470
13	1994	*	C_2-Phenanthrene		2,5-Dimethylphenanthrene	520
14	2109	*	C_3-Phenanthrene + Alkane	205 (100) 57 (93) 43 (86) 71 (60) 220 (56) 85 (42)		
15	2129	*	C_3-Phenanthrene		2,3,5-Trimethylphenanthrene	438
16	2135	*	C_3-Phenanthrene		2,3,5-Trimethylphenanthrene	471
17	2186	**	Pentadecylbenzene	Internal Standard		
18	2206	*	?			
19	2215	*	Phosphate, Trioctyl	57 (100) 70 (98) 41 (68) 55 (66) 100 (50) 83 (40) 112 (38)	Phosphoric Acid, Trioctyl Ester	363
20	2295	*	?	57 (100)	Decane 5,6-Bis(2,2-Dimethyl-Propylidene)	320
21	2367	*	Branched Hydrocarbon C > 21	57 (100) 71 (80) 85 (60) 43 (40)	Docosane	608
22	2396	*	Branched Hydrocarbon C > 23	57 (100)	Docosane, 11-Decyl-	653
			Gas chromatogram looks like a typical gaso	line hydrocarbon mixture.		

TABLE A-3. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 1E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification Before Methylation	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	R.I. x 10³
1	1022	*	Branched Fatty acid (?)	87 (100) 102 (65) 57 (43) 55 (33) 41 (38)	Heptanoic Acid, 2-Ethyl M.E.	440
2	1036	*	?	89 (100) 125 (96) 53 (75) 127 (61) 63 (48) 124 (30)		
3	1160	*	?	133 (100)	Ethanone, 1-(ethylphenlyl)-	223
4	1329	*	?	Poor Mass Spectrum		
5	1685	**	Hexaethylbenzene	Internal Standard		
6	1706	*	Tetradecanoic Acid	74 (100) 87 (50)	Tetradecanoic Acid M.E.	458
7	1887	*	?	41 (100)	10-Undecenoic Acid M.E.	326
8	1913	*	Fatty Acid C ≥14	74 (100) 87 (55)	Pentadecanoic Acid M.E.	638
9	1983	*	Phthalate	149 (100) 41 (18) 71 (6) 150 (10)	1,2 Benzenedicarboxylic Acid Butyl, 2-	469
					Methylpropyl Ester	
10	2073	*	Fatty Acid C ≥17	67 (100)	9,12-Octadecadienoic Acid M.E.	220
11	2083	*	Fatty acid C ≥17	41 (100)	10-Undecenoic Acid M.E.	405
12	2089	*	Fatty Acid C ≥17	55 (100) 69 (69) 79 (62) 87 (33) 41 (60) 43 (48)	11-Octadecenoic Acid M.E.	287
13	2113	1e8	Fatty Acid C ≥18	74 (100)	Tetradecanoic Acid M.E.	652
14	2185	**	Pentadecylbenzene	Internal Standard		
15	2209	*	?	117 (100)	3-Butenoic Acid, 4-Phenyl-butyl Ester	148

TABLE A-4. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 1E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	R.I. x 10³
5	1689	**	Hexaethylbenzene	Internal Standard		
10	1921	*	Phthalate	149 (100)		
					1,2-Benzenedicarboxylic Acid Butyl, 2-	673
11	2183	**	Pentadecylbenzene	Internal Standard	Methylpropyl Ester	

TABLE A-5. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 2VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.11	--	Air	44(100)
2	0.14	1-10	Butene	41(100)56(50)
3	0.16	1-10	Trichlorofluoromethane	101(100)103(66)
4	0.17	1-10	Dichloroethylene	61(100)96(80)98(55)
5	0.17	1-10	Dichloromethane	49(100)51(33)84(85)86(55)
6	0.17	1-10	Carbon Disulfide	78(100)80(6)44( )
7	0.20	1-10	2,3-Dimethylbutane	43(100)42(55)41(39)71(38)57(18)
8	0.20	<1	Butyraldehyde	44(100)72(40)41(25)57(15)
9	0.21	1-10	Methylethyl Ketone	43(100)72(20)57(10)78(7) ?
10	0.21	1-10	3-methylpentane	57(100)56(95)41(95)43(28)86(3)
11	0.23	1-10	Hexane	57(100)41(100)43(80)56(60)86(12)
12	0.26	1-10	Methyl Cyclopentane	56(100)41(65)69(40)84(8)
13	0.27	1-10	1,1,1-Trichloroethane	97(100)99(70)61(60)63(18)117(10)119(8)
14	0.29	<1	Benzene	78(100)51-53(20)
15	0.30	<1	Carbon Tetrachloride	119(100)117(90)47(60)82(50)84(40)121(35)
16	0.31	<1	Cyclohexene	56(100)41(60)84(60)55(45)42(40)
17	0.37	<1	Trichloroethylene	95(100)60(85)40(70)97(60)130(40)132(40)134(40) (Weak)
18	0.55	1-10	Toluene	91(100)92(60)
19	0.88	<1	C_2- Alkyl Benzene	91(100)106(30)92(10)
20	0.91	<1	C_2- Alkyl Benzene	91(100)106(40)105(20)92(10)
21	0.96	<1	Styrene	104(100)78(90)103(70)51(55)77(30)
22	0.98	<1	C_2 Alkyl Benzene	91(100)106(40)105(20)
23	1.00	-(8)	I.S. (Trichloropropane)	75(100)77(33)61(28)
24	1.06	<1	Alkane	43(100)57(90)41(55)85(40)99(10)
25	1.23	<1	Alkane	57(100)41(30)43(30)71(28)85(10)
26	1.24	1-10	C_8H_{12} Hydrocarbon e.g. Vinyl Cyclohexene	54(100)79(65)80(60)107(50)106(30)92(30)
27	1.31	<1	Alkane	57(100)43(90)71(50)85(40)
28	1.51	<1	Alkane + C_4 Alkyl Benzene	57(100)43(73)71(50)41(45)85(28)119(20)134(10)

TABLE A-6. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 2E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification before Methylation	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	RI x 10^3
	1683	**	Hexamethylbenzene	Internal Standard		
1	1710	*	Tetradecanoic Acid	74 (100) 87 (73) 41 (54) 55 (36) 143 (12) 211 (5)	Tetradecanoic Acid M.E.	313
2	1911	*	Hexadecanoic Acid	74 (100) 87 (60)	Pentadecanoic Acid, 14 Methyl M.E.	616
3	1921	*	Phthalate, Dibutyl	149 (100)	1,2-Benzenedicarboxylic Acid	519
					Butyl 2-methyl propyl ester	
4	1987	*	?	Weak Spectra		
5	2071	*	Alkenoic acid C > 18	67 (100)	9,11-Octadecadienoic Acid M.E.	423
6	2082	*	Alkenoic Acid C ≥ 18	55 (100)	10-Octadecenoic Acid M.E.	642
7	2111	*	?	171 (100) 191 (100) 91 (91) 221 (87) 89 (83) (Mixture)	Tridecane, 2 methyl-2 phenyl	209
8	2121	*	Branched alkane acid C ≥ 18	74 (100) 87 (70) 55 (35) 143 (16) 179 (5)	Heneicosanoic Acid M.E.	403
9	--	--				
10	2139	*	Subst. Cyclohexane Acid	146 (100) 101 (68) 136 (63) 91 (52) 41 (46) 92 (42) 187 (48)	Cyclohexanecarboxylic Acid 1,3-Dimethyl-2-	310
					[2-[3-(1-Methyl Ethyl) Phenyl] Ethyl]-M.E.	
11	2150	*	Subst. Cyclohexane Acid	166 (100) Weak Spectra	Ditto	317
12	2170	**	Pentadecylbenzene	Internal Standard		
13	2181	**	Subst. Phenanthrene Acid	59 (100) 41 (83) 91 (71) 67 (70) 241 (54) 262 (44) 302 (10) 121 (100)	Subst.-Phenanthrenecarboxylic Acid M.E.	343
14	2197	*	Subst. Phenanthrene Acid	121 (100) 91 (33) 55 (29) 59 (28)	Subst.-Phenanthrenecarboxylic Acid M.E.	369
15	2210	*	Subst. Phenanthrene Acid	121 (100)	Subst.-Phenanthrenecarboxylic Acid M.E.	369
16	2228	*	Subst. Phenanthrene Acid	41 (100) Weak Spectra	Subst.-Phenanthrenecarboxylic Acid M.E.	200
17	2267	*	Subst. Phenanthrene Acid	41 (100) 81 (92) 91 (90) 105 (90) 79 (88) 241 (36) 242 (33)	Subst.-Phenanthrenecarboxylic Acid M.E.	312
18	2304	**	Subst. Phenanthrene Acid	239 (100) 59 (78) 43 (67) 41 (63) 260 (58)	Subst.-Phenanthrenecarboxylic Acid M.E.	587
19	2360	**	Subst. Phenanthrene Acid	41 (100)	Subst.-Phenanthrenecarboxylic Acid M.E.	287
20	2527	*	Subst. Phenanthrene Acid	59 (100) 253 (85) 254 (78) 187 (69) 211 (46) 213 (46) 329 (18)	5,8,11-Heptadecatriynoic Acid M.E.	218

TABLE A-7. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 3VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.11	--	Air	44(100)40(2)
2	0.12	--	Dimethylether	45(100)46(45)
3	--	--	Air	44(100)40(5)
4	0.13	10-100	Dimethylether	45(100)46(60)
5	0.17	10-100	Dichloroethylene	96(100)61(95)98(70)63(60)
6	0.17	10-100	Dichloromethane	49(100)84(80)86(55)51(25)
7	0.20	1-10	2,3-Dimethylbutane	43(100)42(45)71(30)41(15)
8	0.21	1-10	Methylethyl ketone	43(100)72(30)
9	0.23	10-100	Hexane	57(100)43(60)56(45)41(40)83,85,80(12)
10	0.26	1-10	Methyl cyclopentane	56(100)69(60)41(35)84(10)
11	0.27	10-100	1,1,1-Trichloroethane	97(100)99(66)61(60)63(20),117(10)
12	0.37	1-10	Trichloroethylene	95(100)97(70)130(90)132(85)
13	0.55	1-10	Toluene	91(100)92(60)
14	1.00	-(8)	I.S.	75(100)110(60)112(45)
15	1.02	1-10	Alkane	57(100)56(45)71(20)85(18)
16	1.06	<1	Alkane	71(100)43(60)57(50)113(22)
17	1.11	<1	Alkane	57(100)43(50)41(30)70(22)71(20)98(15)
18	1.23	1-10	Alkane	57(100)71(25)85(20)
19	1.25	<1	Alkane	57(100)56(55)41(32)71(18)85(20)99(10)

TABLE A-8. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 4VI-a

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.12	--	Air	44(100)
2	.13	1-10	Dimethylbutane	41(100)56(62)39(58)
3	.14	1-10	Chloroethane	64(100)66(35)49(15)
4	.15	1-10	Acetone + Dimethyl ether (T)	45(100)43(65)46(35)58(20)
5	.16	<1	Unknown (very weak)	59(100)110(98)108(96)74(60)
6	.16	20-30	Dichloromethene	49(100)84(67)
7	.17	1-10	Methylethyl ketone	43(100)41(83)72(90)
8	.18	1-10	Crotonaldehyde	41(100)39(85)70(92)
9	.22	1-10	Chloroform	83(100)85(66)
10	.22	1-10	Di-n-propoxy ethane	45(100)43(40)87(12)
11	.23	<1	Chlorobutene	55(100)90(50)92(12)
12	.23	1-10	Chlorobutene	55(100)39(50)90(35)92(10)
13	.24	1-10	Tetrahydrofuran	42(100)41(72)71(53)72(52)
14	.24	1-10	1,2-Dichloroethane	62(100)49,64(32)98(10)100(8)
15	.32	10-20	Dichloropropane	63(100)62(70)41(35)76(32)
16	.38	1-10	C_7H_{16}	43(100)71(70)57(60)100(20)
17	.51	1-10	Toluene	91(100)92(62)
18	1.00	8	I.S.	75(100)110(33)
19	1.06	1-10	Diethyl disulfide	66(100)122(90)94(65)
20	1.14	1-10	1-Bromo-2,3-dichloro propane	111(100)75(75)113(65)77(25)124(10)

TABLE A-9. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 4VI-6

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.14	--	Air	44(100)
2	.15	1-10	Chloromethane	50(100)44(34)57(30)
3	.16	1-10	1,3-Butadiene	39(100)54(60)53(45)
4	.17	1-10	Unknown	56(100)55(72)
5	.17	10-100	Acetone	43(100)58(25)44(25)
6	.18	≈10	Chloropropene	41(100)39(85)76(30)59(20)78(8)
7	.19	~10	Dichloromethane	84(100)49(98)
8	.	1-10	Carbon Disulfide	76(100)44(28)78(8)
9	.23	1-10 ea	Chloroform + Alkane	41(100)57(96)43(80)83(78)85(50)130(12)
10		1-10	Tetrahydrofuran	42(100)72(30)71(29)
11		1-10	Vinylchloride (T)	62(100)64(33)35(10)
12	.29	1-10	Benzene	78(100)
13	.35	1-10	Trichloroethylene	95(100)44(87)130(70)132(68)97(62)
14	.54	1-10	Toluene	91(100)92(60)
15	.66	1	Tetrachloroethylene	166(30)129(29)131(27)164(24)
16	.89	1	Ethyl benzene	91(100)106(30)
17	.93	1	Xylene	91(100)106(30)
18	1.00	(-)18	I.S.	75(100)110(30)

TABLE A-10. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 4VF

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.12		Air	44(100)
2	0.19	10-100	Dichloromethane	49(100)84(62)86(40)
3	0.25	10-100	Chloroform	83(100)85(70)87(12)
4	0.28	<1	C_6H_{12}, e.g., Hexane or Methylcyclopentane	56(100)41(60)69(38)84(5)
5	0.29	<1	Trichloroethane	97(100)61(70)99(70)63(20)
6	0.31	<1	Benzene	78(100)
7	0.32	<1	Carbon tetrachloride	119(100)117(95)82(40)47(40)
8	0.38	1-10	Bromodichloromethane	83(100)85(60)47(25)127(8)129(10)131(5)
9	0.56	1-10	Toluene	91(100)92(60)
10	0.60	1-10	Dibromochloromethane	129(100)127(80)13(30)79,81(25)
11	0.88	1-10	C_2 Alkyl benzene	91(100)106(30)
12	0.89	<1	Bromoform	173(100)171(50)175(48)254(10)
13	0.91	1-10	C_2-Alkyl benzene	91(100)106(45)
14	0.98	1-10	C_2-Alkyl Benzene	91(100)106(40)
15	1.00	-(8)	I.S.	75(100)77(30)
16	1.07	<1	C_3-Alkyl benzene	105(100)120(30)
17	1.15	1-10	C_3-Alkyl benzene	91(100)120(25)
18	1.17	1-10	C_3-Alkyl benzene	105(100)120(30)
19		<1	C_3-Alkyl benzene	105(100)120(40)

TABLE A-11. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 4I-a

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	R.I. x 10^3
1	852	*		65(100)78(86)91(74)63(71)92(45)117(32)89(35)131(12)		
6	882	*	?	43(100)59(56)101(61)49(36) Poor spectra		
7	896	*	?	43(100)59(53)101(22)52(20)78(15) Poor Spectra		
10	958	*	?	85(100)43(99)58(65)59(31)115(22)131(18)		
11	986	*	?	85(100)43(99)45(78)58(41)		
13	1030	*	?	57(100)85(88)41(42)93(36)63(32)105(26) Poor spectra		
14	1040	*	?	69(100)68(49)56(35)41(32)78(18)		
15	1138	***	Ethyl Benzenemethanol	107(100)79(58)77(35)105(13)136(8)51(7)	Benzenemethanol,alpha-Ethyl-	625
16	1146	*	1-Phenyl-1-Propanone	105(100)77(43)134(11)51(10)	1-Propanone,1-Phenyl-	672
21	1340	*	?	71(100)43(67)40(28)83(25)56(24)55(23)89(20)98(18) Poor spectrum	1-Hexanol,5-Methyl-	257
22	1356	*	?	71(100)43(70)56(64)89(59)163(12)173(11)	1-Butanol,4-(Hexyloxy)-	279
25	1921	*	Phthalate, Dibutyl	149(100)150(9)106(8)41(7)76(5)205(2)	1,2-Benzenedicarboxylic acid, Butyl-2-Methyl Proply Ester	495
26	2182	**	Pentadecylbenzene	Internal standard		
*	1682	**	Hexamethylbenzene	Internal standard		

TABLE A-12. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 4I-b

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	R.I. x 10^3
1	983	**	1,1'-Oxy Bis [2-Ethoxy]-Ethane (Carbitol)	45(100)59(38)72(31)43(23)104(5)	Ethane 1,1' Oxy Bis[2-Ethoxy]	611
4	1125	*	Acenaphthalene 1,2 Dihydro	154(100)153(35)152(25)155(12)76(13)63(7)51(8)	Acenaphthylene,1,2-Dihydro	608
5	1267	*	Benzenesulfonic Acid 4-Methyl Hydrazide	91(100)152(41)65(33)186(30)	Benzenesulfonic acid 4-methyl hydrazide	196
8	1373	*	Benzenesulfonamide N,4-Methyl	91(100)155(23)65(27)121(23)185(23)	Benzenesulfonamide N,4-Dimethyl	426
9	1645	*	Fatty Acid C≥14	74(100)87(58)43(21)41(18)143(13)		
10	1678	*	Sub anthracene acid	253(100)91(30)254(28)77(23)195(20)		
14	2087	*	Fatty Acid C≥17	55(100)74(86)87(58) Poor MS		
15	2112	*	Octadecanoic Acid	74(100)87(63)44(33)163(11)199(2)	Heneicosanoic Acid M.E.	532
16	2182	**	Pentadecylbenzene	Internal Standard		
*			Palmitic Acid	Internal Standard		

TABLE A-13. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 4I-b

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	K.I. x 10^3
1	873	*	?	83(100)62(50)41(67)56(63)69(27)97(17)	7-Oxabicyclo[4.1.0.]Heptane	560
2	881	*	?	85(100)63(53)58(48)131(22)115(21)71(20)105(7)145(2)	Ethane,(2-Ethoxy-1-Methoxyethoxy)-	252
3	920	*	?	85(100)57(80)41(32)58(22)93(16)162(13)127(8)	3-Pentanone,2,2,4,4-Tetramethyl-	536
4	982	*	?	69(100)68(49)56(36)41(33)62(22)117(7)121(3)		
5	1020	*	2-Bromocyclohexanol	81(100)57(61)99(28)79(18)132(6)178(2)180(1)	Cyclohexanol,2-Bromo-,Cis-	464
6a	1135	**	1-Phenyl-1-propan-1-one	105(100)77(52)51(18)136(10)		
6b	1135		2-Ethyl, Benzenemethanol	107(100)79(61)51(13)136(8)		
11	2180	**	Pentadecylbenzene	Internal standard		
*	1682	**	Hexamethylbenzene	Internal Standard		

TABLE A-14. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 4E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Bieman Match	
					Compound	RI. x 10³
1	857	**c	Unresolved peak	41(100)83(74)42(63)49(52)70(43)97(11)98(8)		
2	878	*	?	55(100)70(92)42(78)98(43)41(48)69(40)		
3	886	**	Chlorocyclohexene	81(100)79(75)80(43)41(32)53(31)116(10)118(4)		
4	1003	**	4-Chlorocyclohexanol	57(100)80(77)44(77)41(70)81(48)88(33)98(23)134(8)136(3)		
5	1015	*	?	41(100)57(91)43(71)55(58)70(32)83(27)		
6	1022	*	Alkyl-cyclohexane	57(100)41(71)43(53)56(35)70(23)83(18)112(2)		
7	1037	***	Dichlorocyclohexane	81(100)80(70)41(28)152(1)		
8	1077	**	2-Bromocyclohexanol	81(100)57(85)41(42)99(27)132(3)178(1)180(1)		
9	1118	***	Bromo,chlorocyclohexane	79(100)81(98)53(85)41(78)51(42)117(36)119(13)	Cyclohexane,1-Bromo-2-Chloro	260
10	1135	*	1-Phenylpropan-1-one	105(100)77(60)51(30)134(12)	1-Propanone,1-Phenyl	647
11	1194	*	1,3-Dibromocyclohexane	81(100)41(21)79(23)161(10)163(10)	Cyclohexene,1,3-Dibromo	406
12	1243	*	Dibromocyclohexane	81(100)41(28)79(23)117(12)244(3)246(1)	Cyclohexane,1,Bromo-2-Chloro	338
13	1264	*	Dihydro indenone (1)	104(100)132(93)78(59)103(53)51(39)131(27)	1-H-Inden-1-one,2,3-Dihydro	417
14	1269	*	Mixture? Bromo?	97(100)41(82)79(79)57(43)69(42)132(39)134(37)198(2)		
15	1288	*	Ethanone,1-(2,4-Dimethylphenyl)	133(100)105(61)77(31)148(28)79(25)	Ethanone,1-(2,4-Dimethylphenyl)-	635
16	1315	*	?	117(100)146(86)118(52)115(42)91(31)43(30)	1-H-Indene,1-Ethyl-2,3-Dihydro	449
17	1333	**	1(2H)-Naphthalenone,3,4-Dihydro	118(100)90(100)146(67)89(60)63(33)51(25)	1(2H)-Naphthalenone,-3,4-Dihydro	613
18	1353	*	C_2-Alkyldihydroindene	117(100)146(62)118(55)115(37)91(30)63(20)	1-H-Indene-1-Ethyl-2,3-Dihydro	488
19	1367	*	C_2-Alkyldihydroindene	117(100)146(75)118(50)115(37)91(34)63(32)167(18)	?	479
20	1369	*	Alkyl naphthalene	118(100)90(95)167(88)160(60)165(55)103(50)77(58)	1(2H)-Naphthalene-3,4-Dihydro-2-Methyl	233
21	1441	*	?	104(100)77(84)132(59)51(59)160(55)41(58)213(48)211(47)264(3)		
22	1458	*	?	165(100)57(92)41(60)180(52)137(51)234(9)236(5)	?	
23	1467	*	?	117(100)115(78)213(67)211(66)226(22)228(21)		
24	1508	*	?	118(100)117(95)115(92)90(58)180(53)246(2)248(3)		
25	1520	*	?	196(100)125(54)198(62)160(36)276(5)278(10)280(4)		
26	1557	*	?	115(100)117(98)224(68)226(66)196(19)198(17)		
27	1591	*	?	118(100)90(58)115(52)144(40)224(8)226(7)		
28	1602	*	?	115(100)117(91)63(43)226(39)224(38)292(9)294(5)		
29	1628	*	?	117(100)242(96)126(88)161(61)240(72)224(50)226(49)		
30	1650	*	?	115(100)117(92)224(62)226(68)129(75)91(56)290(3)293(4)		

TABLE A-14. (Continued)

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	E.I. x 10^3
31	1682	**	Hexaethylbenzene	Internal Standard		
32	1703	*	Mixture HC C ≥ 17	211(100)213(99)57(100)115(85)117(83)292(85)290(42)299(37)		
33	1713	*	?	211(100)213(95)115(90)117(81)292(65)290(40)294(35)91(63)		
34	1899	*	Nonadecane	43(100)57(98)71(63)41(58)85(43)	Heptadecane,2-Methyl	626
35	1921	*	Phthalate, Dibutyl	149(100)101(31)85(25)103(31)		
36	1958	*	Halo alkane +?	55(100)101(43)135(38)87(31)103(28)151(30)	Cl_6-F_6-Pentene	358
37	2000	*	Eicosane +?	43(100)57(93)71(61)85(61)41(48)	Pentacosane	523
38	2101	*	Heneicosane	57(100)43(77)71(62)85(41)55(37)41(33)	Heptadecane,9-Hexyl	568
39	2141	*	Branched Hydrocarbon C ≥ 21	57(100)43(46)71(58)85(33)55(33)	Eicosane-7-Hexyl	551
40	2155	*	?	Peak unresolved on GC-MS		
41	2166	*	?	"		
42	2183	**	Pentadecylbenzene	Internal Standard		
*		**	High boiling Hydrocarbons			
		**	Quantification data unreliable because			
			of increased baseline in GC			

TABLE A-15. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 5VE

GC Peak No	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.13	--	Air	44(100)
2	0.17	<1	Butene	41(100)56(40)
3	0.19	10-100	Acetone	43(100)58(35)
4	0.20	1-10	Dichloromethane	49(100)84(60)
5	0.24	<1	2,3-Dimethylbutane	43(100)42(60)71(10)
6	0.25	<1	3-Methylpentane (T)	57(100)56(90)41(80)
7	0.26	1-10	Hexane (T)	57(100)41(80)43(60)56(50)
8	0.29	1-10	Methyl cyclopentane	56(100)41(50)69(40)84(6)
9	0.57	1-10	Toluene	91(100)92(50)
10	1.00	-(8)	I.S.	75(100)
11	1.19	<1	C_3 Alkyl benzene	105(100)120(45)
12	1.20	1-10	C_3 alkyl benzene	105(100)120(40)
13	1.22	1-10	Alkane	57(100)71(30)85(15)
14	1.24	1-10	C_3 Alkyl benzene	105(100)120(45)
15	1.30	1-10	C_3 Alkyl benzene	105(100)120(40)
16	1.32	1-10	Propenyl benzene	117(100)118(50)115(40)
17	1.36	1-10	C_4 Alkyl benzene	105(100)119(95)134(50)91(32)
18	1.36	1-10	C_4 Alkyl benzene	105(100)134(25)
19	1.37	1-10	C_4 Alkyl benzene	105(100)91(30)119(30)134(30)
20	1.38	1-10	C_4 Alkyl benzene	119(100)134(30)
21	1.39	1-10	C_4 Alkyl benzene	105(100)134(20)
22	1.39	1-10	C_4 Alkyl benzene	119(100)134(30)
23	1.42	1-10	C_4 Alkyl benzene	119(100)134(20)
24	1.43	1-10	C_4 Alkyl benzene	119(100)134(20)
25	1.44	1-10	C_4 Alkyl benzene	119(100)134(20)
26	1.46	1-10	C_4 Alkyl benzene	119(100)134(20)
27	1.49	1-10	C_4 Alkyl benzene	119(100)134(20)
28	1.49	10-100	C_4 Alkyl benzene	119(100)134(20)
29	1.52	1-10	$C_{10}H_{14}$, e.g., (2-Methylpropyl) benzene	117(100)117(40)

TABLE A-15. (Continued)

GC Peak No.	Relative Retention Time	Amount, µg/ℓ	Tentative Identification	Characteristic Ions in Mass Spectrum
31	1.53	1-10	$C_{10}H_{12}$	117(100)132(40)
32	1.54	1-10	C_5 Alkyl benzene	119(100)91(30)148(10)
33	1.54	1-10	C_5 Alkyl benzene	119(100)134(40)
34	1.55	1-10	$C_{10}H_{12}$ (1,2,3,4-Tetrahydro-Naphtralene	104(100)91(40)132(40)
35	1.57	1-10	C_5 Alkyl benzene	119(100)133(50)148(30)
36	1.58	1-10	Naphthalene	128(100)127(15)
37	1.59	1-10	C_5 Alkyl benzene	119(100)148(20)
38	1.63	1-10	C_5 Alkyl benzene	133(100)148(30)
39	1.64	1-10	C_5 Alkyl benzene	133(100)148(20)

TABLE A-16. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 5E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	R.I. x 10^3
2	887	*	?	42(100)41(48)70(32)86(28)97(18)98(15) Poor mass spectra		
3	899	**	Nonane			
6	1002	*	Decane			
10		*				
13	1073	**	2-Bromocyclohexenol	81(100)57(52)99(24)134(5)132(4)180(2)178(1)	Cyclohexanol,2-Bromo	432
14	1085	*	?	Poor spectra	Benzene,2-Ethyl,2,4-Dimethyl	264
15	1098	*	Hydrocarbon Undecane			
16	1101	*	C_4 Alkylbenzene	119(100)134(37)91(23)207(5)	Benzene,tetramethyl	376
17	1111	**	1-Bromo-2-Chlorocyclohexene	81(100)79(22)117(12)53(10)196(3)198(2)200(1)	Cyclohexene,1-Bromo-2-chloro	525
18	1116	*	C_5-Alkylbenzene	107(100)105(49)132(40)148(20)105(19)	Benzene(2-Methyl-1-Propenyl)	393
19		*	?	106(100)132(38)91(29)78(22)	1H-Indene-1,2-Diol,2,3-Dihydro	423
20		*	Naphthalene	128(100)102(11)51(8)	Azulene	326
21		*	C_5-Alkylbenzene	133(100)134(45)91(43)148(40)105(32)104(24) Poor spectra	Benzene,Pentamethyl-	255
22	1210	*	Dibromocyclohexene	81(100)127(51)79(30)112(29)244(5)	Cyclohexane,1,3-Dibromo-	165
23	1289	*	?	132(100)117(87)115(45)91(41)146(29)150(25)214(6)212(5)		
24	1323	*	C_2-Alkyldihydronaphthalene	130(100)120(83)119(82)147(54)91(52)148(43)	Ethanone,1-(2,4,6-Trimethylphenyl)-	344
26	1354	*	1(2H)-Naphthalenone,3,4-Dihydro	118(100)146(63)90(48)89(26)	1(2H)-Naphthalenone,3,4-Dihydro-	450
27	1460	*	?	107(100)125(67)79(42)77(41)136(37)152(26)		
28	1628	*	Tributyl Phosphate	99(100)155(23)125(10)211(8)41(9)57(6)	Phosphoric acid tributyl ester	591

TABLE A-17. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 6VE

GC Peak No.	Relative Retention Time	Amount, μg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.12		Air	44(100)
2	0.18	10-100	Dichloromethane	49(100)84(80)
3	0.22	<1	2,3-Dimethylbutane	43(100)42(50)41(40)71(20)
4	0.23	<1	3-Methylpentane	57(100)56(90)41(90)
5	0.24	1-10	Chloroform + C_6 Alkane	41(100)57(95)43(82)83(60)
6	0.25	1-10	Isopropyl ether	45(100)43(28)87(25)102(7)
7	0.27	1-10	1,2-Dichloroethane	62(100)64(33)49(25)98(8)100(6)
8	0.36	1-10	1,2-Dichloropropane	63(100)41(75)62(70)76(50)97(5)112(3)
9	0.56	1-10	Toluene	91(100)92(60)
10	1.00	(8)	I.S.	75(100)77(33)

TABLE A-18. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 6E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10^3
1	881	*	3-Heptanone	57(100)41(35)85(20)72(15)43(15)114(6)	3-Heptanone	674
2	895	*	?	85(100)43(98)45(90)58(63)71(26)115(15)131(15)	2-Pentanone,3-methoxy	321
3	915	*	?	45(100)43(83)85(68)42(48)57(35)61(25)	"	480
4	957	*	?	57(100)85(78)41(52)93(48)142(12)	3-Pentanone,2,2,4,4-Tetramethyl	262
5	983	*	?	69(100)41(76)68(50)42(46)56(41)121(3)	Propanenitrile,2-Methyl	506
6	1060	*	Acetophenone	105(100)77(90)51(42)120(23)43(20)50(20)	Ethanone,1-Phenyl	706
7	1095	*	Isophorone	82(100)138(16)56(18)41(14)	2-Cyclohexen-1-one,3,5,5-Trimethyl	547
8a	1137	***	1-Phenyl-1-Propanone	105(100)77(80)51(43)39(21)134(10)	Benzenemethanol Ethyl	485
8b	1137		α-Ethyl Benzenemethanol	107(100)79(88)77(52)51(15)136(10)		
9	1151	*	?	81(100)105(83)77(52)41(48)99(10)148(6)		
10	1158	*	?	41(10[illegible])55(83)99(62)114(63)69(62)	2-Propenoic Acid,2-Methyl Pentyl Ester	358
11	1225	*	HC + ?	70(100)41(80)55(71)42(43)69(39)112(16)	2-Octene	738
12	1340	*	?	63(100)71(83)41(40)83(25)	Butane,2,2'-(Methylenebis(oxy)Bis-2-Methyl)	353
13	1355	*	?	43(100)71(96)56(70)89(58)41(50)143(5)173(5)	1-Butanol,4-(Hexyloxy)	522
14	1432	*	?	73(100)41(60)55(50)88(47)101(38)119(17)174(5)		
15	1681	**	Hexamethylbenzene	Internal Standard		
16	1920	*	Phthalate, Dibutyl	149(100)41(20)76(10)205(3)	1,2-Benzenedicarboxylic acid,butyl-2-methylpropyl ester	532
17	2181	**	Pentadecylbenzene	Internal standard		
18	2458	*	Alkyl Benzene	91(100)113(18)57(17)71(12)		
19	2512	*	Phthalate, Bis(2-ethylhexyl)	149(100)57(43)71(30)167(28)	1,2-Benzenedicarboxylic acid-Diisooctyl Ester	363
20	2744	*	?	59(100)55(72)72(73)43(60)(41)60 281(2)	9-Octadecenamide	501
21	2807	*	Alkylpolyene	69(100)81(55)61(42)95(15)	Tetracosahexaene-Hexamethyl-	516

TABLE A-19. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 7VI

GC Peak No	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.12		Air	44(100)
2	0.18	10-100	Dichloromethane	49(100)84(50)
3	0.21	1-10	2,3-Dimethylbutane	43(100)42(55)41(50)71(30)
4	0.22	1-10	3-Methylpentane	57(100)41(90)56(88)71(6)86(4)
5	0.24	1-10	C_6 Alkane + Chloroform	57(100)41(95)43(70)56(55)83(30)
7				44(100)45(90)41(40)43(32)
8	0.27	1-10	Methyl cyclopentane	56(100)41(55)69(40)84(6)
9	0.28	1-10	Trichloroethane	97(100)99(70)61(50)119(10)117(8)
11	0.56	1-10	Toluene	91(100)92(60)
12	1.00		I.S.	75(100)110(50)77(33)
13	1.26	10-100	Dichlorobenzene	146(100)148(70)111(33)113(12)
14	1.27	10-100	Dichlorobenzene	146(100)148(70)111(35)113(10)

TABLE A-20. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 7VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	--	--	Air	44(100)
2		10-100	n-Pentane	43(100)42(95)41(90)57(22)72(12)
3		1-10	Dichloroethylene	61(100)96(60)98(40)63(35)100(4)
4		1-10	Dichloromethane	49(100)84(98) Sat'd
5		<1	2,3-Dimethylbutane	43(100)42(58)41(48)71(20)
6		<1	3-Methylpentane	41(100)57(90)56(80)43(28)71(4)86(2)
7		<1	Chloroform	83(100)85(62)57(40)
8		1-10	Isopropyl ether	45(100)43(33)87(25)102(2)
9		1-10	Methyl cyclopentane	56(100)41(62)69(40)84(8)
10		1-10	Trichloroethane	97(100)99(62)61(55)117,119,121
11		1-10	Carbon tetrachloride	119(100)117(95)121(40)82(40)
12		1-10	Toluene	91(100)92(55)
13		1-10	n-Butyl ether	57(100)41(31)87(25)130(2)
14		10-100	Dichlorobenzene	146(100)148(70)111(45)113(15)
15		10-100	Dichlorobenzene	146(100)148(65)111(50)113(18)

TABLE A-21. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 7I

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10^3
5	985	*	1,3-Dichlorobenzene	146(100)148(61)111(48)75(22)50(13)113(13)150(10)	Benzene,1,3-Dichloro-	588
6	991	*	1,4-Dichlorobenzene	146(100)148(63)111(57)75(30)50(18)113(10)150(11)	Benzene,1,4-Dichloro-	566
8	1016	**	1,2-Dichlorobenzene	146(100)148(65)111(43)75(28)50(15)113(11)150(11)	Benzene,1,2-Dichloro-	652
9	1098	*	Isophorone	82(100)138(22)54(16)95(11)67(9)	2-Cyclohexen-1-one,3,5,5-Trimethyl	289
10	1100	*	Undecane	57(100)43(86)71(50)	Butane,2,2-Dimethyl-	564
11	1136	*	1,2,3,4-Tetrahydronaphthalene	106(100)132(39)91(30)115(18)117(13)78(12)	Naphthalene,1,2,3,4-Tetrahydro-	512
12	1156	*	Naphthalene	128(100)127(21)102(15)129(13)	Naphthalene	340
13	1300	*	Tridecane			
14	1325	*	C_2-Alkyldihydronaphthalene	130(100)119(75)120(74)129(65)91(60)105(53)128(39)	Benzene,1,4-Dimethyl-2-(2-Methyl Propyl)	268
15	1331	**	1(2H)-Naphthalene,3,4-Dihydro	118(100)146(59)90(51)89(25)63(11)147(6)	1(2H)-Naphthalenone,3,4-Dihydro-	662
16	1367	*	1,1'-Biphenyl	154(100)153(40)152(31)	1,1'-Biphenyl	716
17	1368	*	Diphenyl Ether	170(100)141(65)142(42)77(41)51(30)169(29)115(27)171(15)	Benzene,1,1'-Oxybis-	502
18	1682	**	Hexaethylbenzene	Internal standard		
19	2182	**	Pentadecylbenzene	Internal standard		
20	2810	*	Phthalate			
*	1129	*	1-Phenyl,1-Propanone			

TABLE A-22. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 7E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10³
1	887	*	n-Butyl Ether	57(100)41(39)87(13)56(20)101(6)	Butane,1,1'-Oxybis	543
2	905	**	2-Butoxyethanol	57(100)41(73)45(60)87(23)43(18)75(10)	Ethanol,2-Butoxy	877
3	985	*	1,3-Dichlorobenzene	146(100)148(65)111(43)75(43)74(32)50(32)150(10)	Benzene,1,4-Dichloro	509
4	990	*	1,4-Dichlorobenzene	146(100)148(63)111(42)75(41)50(28)150(10)	Benzene,1,2-Dichloro	492
5	1003	1*	?	57(100)43(84)41(67)124(52)62(38)71(30)55(30)		
6	1014	**	1,2-Dichlorobenzene	146(100)148(63)111(51)75(55)50(42)150(10)	Benzene,1,2-Dichloro	429
7	1096	*	Isophorone	82(100)54(21)138(17)41(17)	2-Cyclohexen-1-one,3,5,5-Trimethyl	423
8	1100	*	Undecane	43(100)57(88)41(68)71(40)85(23)		
9	1136	**	1,2,3,4-Tetrahydronaphthalene	104(100)91(47)132(40)78(25)51(20)		
10	1156	*	Naphthalene	128(100)127(13)129(11)102(13)51(13)	Azulene	358
11	1193	*	Alkyl-diketone n-methyl-	57(100)41(93)43(82)58(58)85(55)109(26)127(22)	3-Pentanone,2,2,4,4-Tetramethyl	403
12	1269	*	2-Pentanone,4-Methyl-4-Phenyl	161(100)91(72)119(48)176(41)41(42)43(42)	2-Pentanone,4-Methyl-4-Phenyl	412
13	1331	**	1,2,3,4-Tetrahydronaphthalen-1-one	118(100)90(92)146(65)89(45)63(29)	1-(2H)Naphthalenone,3,4-Dihydro	551
14	1359	*	?	Poor mass spectra (too weak)		
15	1368	*	Diphenyl Ether	170(100)51(70)77(64)141(62)142(41)115(26)	Benzene,1,1'-Oxybis	562
16	1397	**	Phenol,2,4-Bis(1-Methylethyl)-	163(100)121(27)178(23)107(19)91(21)	Phenol,2,4-Bis(1-Methylethyl)-	582
17	1420	*	Ethanol,2-[]-(2-Butoxyethoxy]-	57(100)41(73)45(53)75(28)85(23)	Ethanol,2-[2-(2-Butoxyethoxy)ethoxy]-	458
18	1438	*	Subst. Phenol	163(100)178(38)135(55) Poor spectra	Phenol,2,4-Bis(1-Methylethyl)	251
19	1506	***	2,6-Bis(1,1-Dimethylethyl)-4-methyl pheno	205(100)43(81)41(62)91(32)220(21)177(18)	Phenol,2,6-Bis(1,1-Dimethylethyl-4-methyl	218
20	1554	*	Alkyl Benzene	43(100)41(76)91(40) Poor spectra		
21	1588	**	Isomer of #19	205(100)43(83)41(58)220(21)	Phenol,2,4-Bis(1-Methylbutyl)-	330
22	1630	**	Tributyl Phosphate	99(100)41(28)155(12)211(5)	Phosphoric Acid Tributyl Ester	499
23	1657	*	?	195(100)165(23)196(16)210(8)	Naphthalene,1,2,3-Trimethyl-4-Propenyl	236
24	1682	**	Hexamethylbenzene	Internal standard		
25	1690	*	Phthalate	41(100)149(40)71(23)104(18)189(8)	1,2-Benzenedicarboxylic acid-Di-2-Propenyl Ester	332
26	1707	*	?	43(100)205,220 Poor spectra	Phenol,2,4-Bis(1-Methylbutyl)-	187
27	1759	*	?	189(100) Poor spectra		
28	1843	*	?	175(100)94(35)174(30)286(5) Poor spectra		
29	1880	*	?	220(100)237(83)115(92)77(78)	Cinnoline,6-Methyl-4-Phenyl-	195
30	1887	*	Phthalate	[illegible]	1,2-Benzenedicarboxylic acid-butyl-2-	571

TABLE A-22. (Continued)

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10^3
31	1941	*	1,1'-Biphenyl,2-Phenoxy	77(100)246(79)152(68)115(60)51(53)265(18)	1,1'-Biphenyl,2-Phenoxy	354
32	2103	*	?	41(100) 57(100) 125(73)45(70)56(68) Weak Spectra		
33	2145	*	Phenoxy 1,1'-Biphenyl	77(100)246(66)115(60)51(51)141(31)152(23)	1,1'-Biphenyl,2-Phenoxy	261
34	2182	**	Pentadecylbenzene	Internal Standard		
35	2345	**?	Phosphoric Acid, Triphenyl Ester	77(100)51(53)65(53)96(18)169(13)215(10)	Phosphoric Acid,Triphenyl Ester	302
36	2381	**	?	57(100)45(90)41(75)56(58)125(32)		
37	2429	*	Subst. Phosphate	77(100)65(39)51(28)91(27)340(15)339(10)	Carbonic Acid 4-Methyl Phenyl Methyl Ester	304
38	2441	*	Isomer of #35	77(100)322(100)51(35)215(42)226(41)202(38)		
39	2460	*	Phthalate	149(100)167(30)55(18)41(14)249(5)	1,2-Benzenedicarboxylic Acid Dipentyl Ester	290
40	2489	**	Tricresyl phosphate	77(100)118(92)117(46)251(35)368(12)51(33)	Benzene Cyclopropyl-	307
41	2514	*	Phthalate, Bis(2-ethylhexyl)	149(100)163(32)57(23)41(23)43(20)	1,2-Benzenedicarboxylic Acid Diisooctyl Ester	368
42	2540	*	Tricresyl phosphate	77(100)91(62)65(43)165(26)353(20)51(23)	Benzoic Acid,2-Hydroxy-Phenyl Methyl Ester	236
43	2569	*	Tricresyl phosphate	77(100)51(28)91(28)103(24)251(18)353(13)368(7)	Benzene,(1-Methylethynyl)-	265
44	2594	*	Tricresyl phosphate	91(100)65(50)77(42)165(28)368(25)367(17)368(18)410(5)		
45	2614	**	Tricresyl phosphate	77(100)353(52)118(41)51(37)91(36)103(32)65(30)	Benzene,(2-Nitropropyl)	195
46	2638	*	?	77(100)145(91)160(30)43(27)41(24)115(21)	Benzene,1-(1,1-Dimethylethyl)-4-Ethenyl-	338
47	2650	*	Tricresyl phosphate	91(100)77(66)65(44)117(39)368(34)79(33)367(20)		
48	2663	*	?	91(100)77(89)145(68)117(51)160(43)43(40)41(30)251(18)		
49	2676	** 1	Trixylyl phosphate	165(100)77(75)160(57)251(27)91(25)410(15)		
50	2696	**	?	77(100)43(46)41(36)91(30)179(23)160(18)		
51	2736	**	Trixylyl phosphate	91(100)118(95)117(58)103(42)77(38)41(38)43(32)	Benzene, Cyclopropyl	305
52	2757	*	Homolog of #49	165(100)43(50)91(47)160(44)77(44)103(40)107(40)	Naphthalene,1,2,3,4-Tetrahydro-1,1-Dimethyl	264
53	2797	**	Homolog of #49	165(100)77(93)160(78)91(79)103(68)117(68)43(73)	Benzene,1-(1-Methylethenyl)-4-(1-Methylethyl)	226
54	2806	*		145(100)160(46)91(29)115(23)43(23)77(19)	Naphthalene,1,2,3,4-Tetrahydro-1,8-Dimethyl	350
55	2855	**	Homolog of #51	91(100)118(92)43(68)117(63)103(58)77(52)41(48)	Benzene(1-Propyl-1-Nonenyl)	217
56	2863	**	?	165(100)91(63)43(60)160(52)117(48)41(28)115(22)	Naphthalene,1-Butyl-1,2,3,4-Tetrahydro 4-Pentyl	236
57	2868	*		165(100)160(63)43(24)91(16)115(12)77(15)	Benzene,1-(2-Butenyl)-2,3-Dimethyl	359
58	2883	*	Trialkylphenyl phosphate	91(100)165(95)43(70)117(61)160(40)283(23)319(20)		
59	2913	**	?	91(100)43(77)117(61)165(56)160(52)118(50)77(28)		
60	29[illegible]	**				

TABLE A-22. (Continued)

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10^3
61	2972	*	?	43(100)145(97)160(68)91(63)117(46)41(40)77(33)115(35)		
62	2986	*	?	91(100)43(81)103(68)118(55)117(54)77(48)41(42)335(30)319(43)		
63	2995	*	?	43(100)77(99)91(87)115(61)41(63)103(55)107(57)437(23)202(30)		
64	3033	*	?	43(100)145(82)91(75)160(52)117(42)41(42)103(31)118(31)		
65	3080	**	Trialkylphenylphosphate	43(100)145(63)91(61)160(42)117(35)41(35)115(22)105(20)		
66	3101	*	?	145(100)43(96)91(78)160(58)103(40)77(38)41(38)		
67	3113	*	?	91(100)103(80)77(62)43(52)437(38)438(15)41(32)115(28)		
68	3144	*	?	43(100)91(61)107(48)202(36)118(31)41(25)145(21)342(6)		
69	3159	*	?	145(100)43(96)91(77)160(53)319(43)103(43)41(36)77(33)		
70	3205	*	?	43(100)145(90)160(65)91(58)117(34)115(28)105(28)		

TABLE A-23. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 7E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10^3
1	906	**	2-Butoxyethanol	57(100)41(98)45(91)87(27)75(13)100(5)	Ethanol,2-Butoxy	606
3	2181	**	Pentadecylbenzene	Internal Standard		

TABLE A-24. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 8VE

GC Peak No.	Relative Retention Time	Amount, µg[a]	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.11		Air	44(100)
2	0.19	10-100	Dichloromethane	49(100)84(60)
3	0.20	1-10	Chloroform	83(100)85(65)
4	0.26	1-10	Isopropanol	45(100)43(50)41(20)59(6)60(7)
5	0.29	<1	Dichloroethane	62(100)64(30)49(25)98(5)
6	0.38	1-10	Dichloropropane	63(100)41(82)62(70)76(50)
7	0.58	<1	Toluene	91(100)92(60)
8	1.00	~(8)	I.S.	Don't have spectrum.

TABLE A-25. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 8E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	B.I. x 10³
1	836	*	Toluene	91(100)92(68)65(13)63(10)50(7)	Benzene, Methyl	464
2	896	*	3-Heptenone	57(100)85(30)41(23)72(20)114(13)	3-Heptanone	427
3	915	*	?	85(100)57(77)41(77)43(67)71(28)115(23)131(18)	1,3-Dioxane-2-Propanol,2-Methyl	206
4	924	*	?	43(100)85(93)45(78)42(52)58(42)59(40)101(13)	Butanoic acid 3-Hydroxy-3-Methyl Ester	267
5	957	*	4-Octanone	57(100)85(82)41(48)142(13)	4-Octanone,2-Methyl	175
6	983	*	?	69(100)68(52)41(43)54(38)94(6)	Pentanedinitrile	191
7	1023	*	?	57(100)41(40)55(33)56(32)83(18)	Hexanol, 2 Ethyl	612
8	1040	*	Acetophenone	105(100)77(62)120(22)51(23)43(20)	Ethanone,1-Phenyl	692
9	1137	***	1-Phenyl-1-Propanone	105(100)77(49)107(28)79(22)134(8)	p-Propanone,1-Phenyl	530
10	1339	*	?	71(100)43(86)41(36)56(32)83(30)173(2)	Hexene,2,4,5,-Trimethyl	254
11	1355	*	Alcohol C ≥ 11	43(100)71(96)56(78)89(59)41(50)143(5)173(5)	1-Butanol-4-(Hexyoxy)-	584
12	1426	*	Alcohol C ≥ 12	73(100)88(58)101(46)55(37)41(43)119(28)174(8)	1,3-Propanediol,2,2-Dimethyl	224
13	1557	*	Diethyl Phthalate	149(100)177(18)176(10)76(11)104(8)105(9)65(8)	1,2-Benzenedicarboxylic acid diethyl ester	554
14	1682	**	Hexamethylbenzene	Internal Standard		
15	1828	*	Phthalate	149(100)150(9)104(8)57(8)41(12)167(3)223(3)	1,2-Benzenedicarboxylic acid-Butyl-2-Methylproply Ester	596
16	1920	*	Phthalate, Dibutyl	149(100)150(9)104(8)76(5)41(9)121(3)205(2)223(2)	"	699
17	2035		Alcohol	71(100)43(96)67(70)81(70)137(68) Poor Spectra	Cyclotetradecanol,1,7,11-Trimethyl-4-(1-Methylethyl)-	220
18	2082	*	Alcohol (1-Eicosanol)	43(100)55(70)83(70)97(68)41(68)111(26)125(22)	1-Eicosanol	480
19	2181	**	Pentadecylbenzene	Internal standard		
20	2269	**	Phthalate	149(100)104(18)77(12)5712 41(12)133(11)207(8)263(9)	1,2-Benzenedicarboxylic acid,2-Butoxyethyl Butyl Ester	604
21	2410	*	Alkyl Aromatic-Ketone	105(100)163(38)77(27)207(3)	2,4-Pentanedione 3-Ethyl-3-Hydroxy Benzoate	306
22	2422	*	"	105(100)162(52)77(24)207(2)	"	279
23	2488	*	?	99(100)105(35)163(21)113(18)211(3)		
24	2512	*	Alkene	55(100)43(95)41(93)69(63)74(60)96(53)97(50)207(24)	6-Tridecene, Hexam[illegible]yl,7-(trimethyl hexyl)	412
25	2606	*	Phthalate	149(100)112(30)57(16)41(14)207(8)321(5)	1,2-Benzenedicarboxylic acid,2-Butoxy, 2-Oxoethyl Butyl Ester	353
26	2744	*	?	59(100)72(60)43(50)55(43)	1,7-Octanediol,2,7-Dimethyl	303

TABLE A-26. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 9VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.13		Air	44(100)
2	0.16	~100	Acetone	43(100)58(30)
3	0.17	1-10	Dichloroethylene	61(100)63(33)96(35)98(22)
4	0.17	10-100	Dichloromethane	49(100)84(95)
5	0.20	~1	2,3-Dimethylbutane	43(100)42(55)41(40)71(30)86(2)
6	0.21	<1	3-Methylpentane	57(100)56(82)41(70)43(30)
7	0.23	10-100	Chloroform	83(100)85(60)87(10)
8	0.26	<1	Methylcyclopentane	56(100)41(50)69(40)84(10)
9	0.36	10-100	Bromodichloromethane	83(100)85(70)87(10)127,129,131(~7)
10	0.55	1-10	Toluene	91(100)92(60)
11	0.59	1-10	Dibromochloromethane	129(100)127(80)131(30)79,81(20)
12	1.00	-(8)	I.S.	75(100)77(30)110(25)
13	1.51	<1	HC M152	57(100)43(73)71(50)85(30)
14	1.68	<1	Dodecane	57(100)43(70)71(60)85(35) M+170
15	1.71	<1	Alkane	57(100)43(50)43(40)85(15)
16	1.72	<1	M182 Alkene	69(100)55(75)41(55)57(55)83(50)

TABLE A-27. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 9E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Bieman Match	
					Compound	R.I. x 10^3
1	854	**	Toluene	91(100)92(62)65(13)63(8)93(4)50(3)	Benzene, Methyl	470
2			?	129(100)127(82)79(52)81(51)131(25)48(21)47(20)93(14)		
3	880	*	?	83(100)42(56)55(31)69(27)97(13)	Cyclopentanone,2,5-Dimethyl	276
4			?	79(100)81(90)91(80)93(56) Poor Spectrum		
5			?	70(100)83(48)97(47)69(40)98(39)55(38)42(22)	2-Cyclohexen-1-ol	466
6	887	**	Chlorocyclohexene	81(100)79(95)80(50)77(40)53(22)116(18)118(15)	Cyclohexene,2-Chloro	412
7	907	*	?	177(100)175(64)179(45)61(32)96(26)95(25) Poor Spectrum		
8	935	/*	Benzaldehyde	105(100)106(90)77(55)51(29)50(29)	Benzaldehyde	516
9	1002	***	4-Chlorocyclohexanol	57(100)80(29)44(23)81(21)134(5)136(1)	Cyclohexanol,4-Chloro-,Trans-	329
10	1016	*	2-Chlorocyclohexanone	55(100)42(71)132(37)97(36)68(35)88(32)	Cyclohexanone,2-Chloro-	225
11	1037	***	Dichlorocyclohexane	81(100)80(63)79(26)41(18)116(3)152(1)	Cyclohexane,1,2-Dichloro-	336
12	1066	*	?	91(100)65(21)81(19)63(17)92(16)	Benzeneacetic Acid, 2-Propenyl Ester	268
13	1075	** !	2-Bromocyclohexanol	81(100)57(49)99(28)41(23)	Cyclohexanol,2-Bromo-	444
14	1087	*	Dichlorocyclohexane	81(100)80(93)79(60)53(53) Weak Spectra	Cyclohexane,1,2-Dichloro-	321
15	1100	*	Undecane	57(100)43(96)41(62)71(52)56(31)	Heptane,2,2,4-Trimethyl-	275
16	1115	***	Bromo, Chlorocyclohexane	81(100)79(23)117(10)119(4)198(2)196(1)	Cyclohexane,1-Bromo-2-Chloro-,Cis	480
17	1201	*	Dodecane	43(100)71(86)57(82)85(48)81(45)	2-Pentene,1-Ethoxy-4,4-Dimethyl	407
18	1212	*	?	43(100)57(91)71(78)41(60)81(25)98(23)	Hexanal,5-Methyl-	279
19	1216	*	Dibromocyclohexane	81(100)127(61)79(31)117(22)128(13)	Cyclohexane,1,3-Dibromo-	210
20	1265	* !	?	97(100)79(82)43(58)132(57)57(56)134(155)115(41)		
22	1280	*	?	57(100)69(65)71(64)41(59) Poor Spectra		
23	1285	* !	?	71(100)57(78)43(77)113(20)112(19)85(16)	Pentadecane,2,6,10,14-Tetramethyl	395
24	1290	*	?	97(100)55(78)69(77)40(21) Poor Spectra		
25	1301	*	Tridecane	43(100)57(91)71(69)85(48)113(7)112(6)	Dodecane,2,6,11-Trimethyl-	627
26	1319	*	?	57(100)71(75)43(55)44(50) Poor Spectra		
27	1351	*	Alkylcyclohexane	83(100)55(99)43(91)69(81)57(64)82(56)	Cyclohexane, Eicosyl-	310
28	1359	*	?	71(100)43(99)57(85)69(71)55(63) Weak Spectra		
30	1379	*	?	71(100)43(72)57(70)85(40)69(26)	Tetradecane,2,6,10-Trimethyl-	339

TABLE A-27. (Continued)

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10³
31	1400	*.*	Tetradecane	43(100)57(84)71(72)85(53)113(8)112(7)	Tetradecane,2,6,10-Trimethyl	446
32	1405	*	Branched Hydrocarbon C ≥ 14	57(100)44(78)43(70)85(58)71(13) Weak spectra		
33	1464	*	Branched Hydrocarbon C ≥ 14	43(100)71(93)57(72)85(42)113(20)	Tetradecane,2,6,10-Trimethyl	425
34	1501	*	Pentadecane	57(100)71(99)43(92)85(57)41(46)44(39)69(27) Weak Spectra		
35	1682	**	Hexaethylbenzene	Internal standard		
36	1922	**	Phthalate, Dibutyl	149(100)150(10)105(4)76(3)205(2)223(1)	1,2-Benzenedicarboxylic Acid,Butyl-2-Methyl Propyl Ester	561
40	2183	**	Pentadecylbenzene	Internal Standard		
41	2300	*	Phthalate, Butyl Benzyl	149(100)91(50)123(17)206(12)150(15)132(13)		
43	2380	*	?	85(100)125(99)199(53)155(48)153(44)	1,2-Benzenedicarboxylic acid, Dibutyl Ester	208
44	2464	*	Phthalate	149(100)167(33)44(6)	Octadecane,-Hexamethyl-7,12-Bis(3,5,5-Trimethylhexyl)	226
45	2516	*	Phthalate Bis(2-Ethylhexyl)	149(100)167(28)57(12)43(11)113(9)		

TABLE A-28. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 9E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10^3
1	903	**	Toluene	91(100)92(49)65(19)51(6)50(5)	Benzene, Methyl-	461
3	926	**	?	70(100)83(52)55(51)97(40)69(41)43(33)79(27)	Cyclohexanone,2-Propyl-	288
4	965	**	Pentanoic Acid, 3-Methyl	74(100)43(57)59(35)87(32)55(20)99)20)101(9)	Pentanoic Acid,3-Methyl,-Methyl Ester	506
7	995	**	Carbitol	45(100)59(37)43(28)72(23)104(3)103(2)	Ethane,1,1'-Oxybis[2-Ethoxy-]	364
11	1031	**	?	87(100)102(68)53(37)41(29)130(12)129(11)	Heptanoic Acid,2-Propyl,-Methyl Ester	227
12	1035	*	Dichlorocyclohexane	81(100)80(60)79(29)41(23)53(20)62(13)	Cyclohexane,1,2-Dichloro-,Cis-	396
14	1069	**	Benzoic Acid	105(100)77(60)136(22)51(28)50(15)	Benzoic Acid, Methyl Ester	576
15	1111	**	Octanoic Acid	74(100)87(65)43(41)41(32)59(23)127(11)105(9)129(3)	Octanoic Acid, Methyl Ester	406
16	1149	**	Benzeneacetic Acid	91(100)150(29)65(17)59(10)		
20	1512	**	Dodecanoic Acid	74(100)87(63)43(47)41(35)55(29)143(10)171(5)183(2)185(1)	Dodecanoic Acid, Methyl Ester	504
35	1664	**	p-Toluenesulfonamide	91(100)155(25)65(24)185(21)121(19)	Benzenesulfonamide,N,4-Dimethyl-	506
38	1710	**	Tetradecanoic Acid	74(100)87(70)43(42)55(30)143(21)199(9)242(2)243(1)	Tetradecanoic Acid, Methyl Ester	557
40	1809	*	Pentadecanoic Acid	74(100)87(81)43(43)143(23)213(8)	Pentadecanoic Acid, Methyl Ester	475
41	1875	*	Halo Acid (Br)	156(100)74(63)91(53)157(47)406(42)237(40)		
42	1883	*	Fatty Acid C ≥ 15	74(100)87(74)43(60)143(20)129(10)	Decanoic Acid, Methyl Ester	582
43	1916	***	Hexadecanoic acid	74(100)87(78)43(48)55(35)143(21)227(5)271(1)	Hexadecanoic Acid, Methyl Ester	610
48	2010	*	Heptadecanoic Acid	74(100)87(72)43(56)143(20)221(5)199(4)	Heptadecanoic Acid, Methyl Ester	549
52	2114	**	Octadecanoic Acid	74(100)87(81)43(52)55(42)143(27)199(8)299(6)	Octadecanoic Acid,17-Methyl-,Methyl Ester	615
53	2163	*	Impurity ?	43(100)73(60)55(52)60(50)129(35)285(8)		
54	2183	**	Pentadecylbenzene	Internal Standard		
55	2224	*	?	43(100)104(86)98(68)117(42)239(7)	Tetradecanoic Acid,2-Hydroxyethyl Ester	357
56	2245	*	Alkenoic acid C ≥ 18	155(100)55(48)87(42)43(38)74(32)109(31)187(11)206(3)	Octadecanoic Acid,9,10-Dihydroxy-Methyl Ester	423
57	2255	*	C ≥ 19 Alkyl acid	55(100)74(95)	Cyclopropane Pentanoic Acid,2-Undecyl-, Methyl Ester, Trans-	372
58	2266	**	Oxiraneoctanoic acid 2-Octyl	55(100)155(68)43(60)74(54)109(37)97(36)	Oxiraneoctanoic Acid,2-Octyl-,Methyl Ester	346
59	2306	*	Eicosanoic acid	169(100)87(55)43(50)55(42)74(39)201(11)	Tetradecanoic Acid,12-Methyl-,Methyl Ester	295
60	2316	*	Subst. Fatty Acid C ≥ 20	74(100)87(77)43(55)143(27)199(5)284(6)327(3)	Heneicosanoic Acid, Methyl Ester	502
61	2429	*	Subst. Fatty Acid C ≥ 21	43(100)104(74)98(65)41(54)117(40)55(39)155(12)154(8)	Eicosanoic Acid,2-Hydroxy Ethyl Ester	437
62	2451	*	Octadecanoic Acid,9,10-Dihydroxy	155(100)87(54)55(52)43(47)74(34)109(33)206(6)	Octadecanoic Acid,9,10-Dihydroxy-, Methyl Ester	494
63	2472	*	Subst. Fatty Acid (unsat.) C ≥ 22	74(100)43(39)87(33)55(30)		
64	2480	*	Cloro Fatty Acid	74(100)43(43)87(33)55(31)95(18)109(12)	Octadecanoic Acid,9,10-Dichloro-, Methyl Ester	401

TABLE A-29. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 10VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.11		Air	44(100)
2	0.18	<1	Dichloroethylene	61(100)96(70)62(50)98(62)63(15)
3	0.19	1-10	Dichloromethane	49(100)84(100)
4	0.20	<1	[illegible]	69(100)41(60)40(55)42(70)
5	0.25	<1	Chloroform	83(100)85(70)
6	0.27	<1	Tetrahydrofuran	42(100)41(50)72(90)71(38)
7	0.29	<1	Trichloroethane	97(100)99(70)61(60)117,119,121 <(10)
8	0.57	<1	Toluene	91(100)92(60)
9	1.00	(8)	I.S.	75(100)

TABLE A-30. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 10E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Bieman Match	
					Compound	R.I. x 10³
1	860	*	?	83(100)42(68)41(63)55(42)56(41)69(32)97(12)	7-Oxabicyclo[4.1.0]Heptane	414
2	880	*	?	70(100)83(36)69(49)55(48)97(43)98(27)42(36)41(36)79(33)		
3	892	* 13	?	79(100)77(33) Poor spectra		
4	1002	* 1	HC + Chlorocyclohexanol	57(100)80(26)41(22)44(21)88(12)98(9)134(6)116(3)	Cyclohexanol,4-Chloro-,Trans	227
5	1008	*	?	41(100)69(58)43(57)74(31)55(25)		
6	1048	* 3	?	55(100)41(93)57(62)68(33)83(12)	2-Propenoic Acid,2-Propenyl Ester	413
7	1136	*	Chlorocyclohexene	79(100)81(80)53(60)41(38)77(32)97(25)	Cyclohexene,2-Chloro-	286
8	1172	*	Bromocyclohexanol	81(100)127(36)79(27)41(26)57(25)99(24)128(10)	Cyclohexanol,2-Bromo-,Cis-	329
9	1186	* 16	Dibromocyclohexene	81(100)41(62)79(32)55(30)57(27)98(8)		
10	1215	* 18	Bromochlorocyclohexane	81(100)127(33)79(32)53(21)41(17)112(12)128(8)	Cyclohexane,1-Bromo-2-Chloro-,Cis-	375
11	1220	* 1	?	41(100)80(78)77(68)106(65)159(46)91(42)93(35)161(15)		
13	1387	**	Biphenyl	156(100)153(63)152(31)155(16)151(11)76(10)	Acenaphthylene,1,2-Dihydro-	468
14	1897	*	Alkylbenzene	158(100)112(38)91(32)143(27)159(16)168(3)	Benzene,1,3-Bis(1-Methylethenyl)	406
15	2181	**	Pentadecylbenzene	Internal Standard		
*	1679	** 3	Hexaethylbenzene	Internal Standard		

TABLE A-31. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 10E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10^3
1	1137	*	?	79(100)53(90)81(83)61(52)66(61)77(32)97(28)	Cyclohexene,3-(2-Propynyl)-	402
2	1509	*	?	91(100)155(35)186(32)65(31)107(15)122(8)	Benzene,(Ethoxy Methyl)-	427
3	1653	**	p-Toluenesulfonamide	91(100)65(31)155(25)185(21)121(19)	Benzene Sulfonamide,N,4-Dimethyl-	383
4	1672	*	?	163(100)103(96)135(84)165(73)77(41)202(34)169(28)		
5	1708	*	Tetradecanoic Acid	74(100)87(72)143(20)199(8)	Tetradecanoic Acid,Methyl Ester	472
6	1772	*	?	74(100)87(73)43(64)165(23)213(8)157(7)	Cyclopentane undecanoic Acid, Methyl Ester	647
7	1782	**	?	186(100)91(88)103(85)135(69)203(56)163(43)211(8)		
8	1808	*	Pentadecanoic Acid	74(100)87(77)43(41)59(27)143(21)	Dodecanoic Acid, Methyl Ester	253
9	1886	*	?	41(100)55(95)74(78)97(58)96(56)151(24)196(13)236(11)	9-Hexadecenoic Acid, Methyl Ester	466
11	1919	*	?	164(100)150(86)192(68)132(42)234(30)178(25)205(17)		
13	2087	*	Octadecenoic Acid	55(100)74(63)87(48)180(9)195(8)181(5)222(6)	10-Octadecenoic Acid, Methyl Ester	573
14	2110	*	Octadecanoic Acid	74(100)87(72)43(58)143(20)199(5)157(3)	Heneicosanoic Acid, Methyl Ester	726
15	2182	**	Pentadecylbenzene	Internal Standard		
16	2334	*	?	43(100)217(32)275(6)276(5) Poor Spectra		
17	2378	*	?	45(100)217(80)43(66)218(17)170(16)177(13)		
18	2513	*	?	118(100)117(81)91(67)77(58)170(47)171(38)181(15)		
*			Palmitic Acid	Internal Standard		

TABLE A-32. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 11VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.15		Air	44(100)
2	0.19	~10	Dichloromethane	84(100)49(95)
3	0.20	1-10	Carbon disulfide	76(100)78(10)
4	0.26	1-10	Chloroform	83(100)85(70)
5	0.27	1-10	Diisopropyl ether	45(100)43(60)87(30)59(15)
6	0.34	10-100	Carbon tetrachloride	117(100)119(95)121(30)82(28)
7	0.39	10-100	Dichloropropane	63(100)62(68)76(40)41(32)
8	1.00	-(8)	I.S.	75(100)77,110(33)

TABLE A-33. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 12VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.15	-	Air	44(100)
2	0.18	10-100	Acetone	43(100)58(30)
3	0.18	1-10	+ Fluorotrichloromethane	101(80)103(50)105(10)
4	0.19	<1	Diethyl ether +	59(100)45(95)74(55)41(55)76(25)78(10)
5	0.19	<1	Chloropropene	
6	0.19	1-10	Dichloroethylene	61(100)96(50)98(40)63(30)
7	0.19	1-10	Dichloromethane	49(100)84(80)
8	0.20	1-10	Carbon disulfide	76(100)78(15)
9	0.21	<1	2,3-Dimethylbutane	43(100)42(50)41(35)71(20)
10	0.23	<1	Methylethyl ketone	43(100)72(25)
11	0.24	<1	3-Methylpentane	57(100)56(95)41(88)
12	0.25	1-10	Chloroform	83(100)85(60)
13	0.27	1-10	Tetrahydrofuran	42(100)41(60)71(30)72(30)
14	0.28	1-10	Dichloroethane	62(100)64(32)49(30)98(5)
15	0.29	<1	1,1,1-Trichloroethane	97(100)99(70)61(40)119(15)
16	0.31	1-10	Benzene	78(100)
17	0.37	1-10	1,2-Dichloropropane	63(100)62(72)41(68)76(40)
18	0.37	<1	3-Pentanone	57(100)86(20)
19	0.38	<1	Bromodichloromethane	83(100)85(65)129(10,127(8)131(3)
20	0.38	<1	Trichloroethylene	95(100)130(90)132(88)97(70)
21	0.54	1-10	1,1,2-Trichloroethane (T)	97(100)83(80)99(70)61(60)85(50)63(25) (Weak)
22	0.56	1-10	Toluene	91(100)92(60)
23	0.88	<1	C_2 Alkyl benzene	91(100)106(30)
24	0.91	<1	C_2 Alkyl benzene	91(100)106(40)
25	0.98	<1	C_2 Alkyl benzene	91(100)106(40)
26	1.00	-(8)	I.S.	75(100)77(33)110(30)
27	1.06	<1	Alkane	71(100)43(60)57(55)
28	1.06	<1	Alkane	43(100)57(90)
29	1.17	<1	C_3 Alkyl benzene	105(100)120(30)
[illegible]	1.18	<1	C_3 Alkyl benzene	105(100)120(30)

TABLE A-33. (Continued)

GC Peak No	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
11	1.19	<1	C_3 Alkyl benzene	105(100)120(40)
12	1.20	<1	C_{10} Branched alkane	57(100)85(65)41(40) 142 M
13	1.21	<1	C_3 Alkyl benzene	105(100)120(30)
14	1.22	<1	Branched alkane	57(100)56(35)
15	1.25	<1	C_3 Alkyl benzene	105(100)120(35)
16	1.26	<1	Dichlorobenzene	146(100)148(70)
17	1.27	<1	Branched alkane	57(100)56(40)
18	1.30	<1	C_3 Alkyl benzene	105(100)120(15)
19	1.37	<1	C_4 Alkyl benzene	105(100)134(20)
20	1.38	<1	C_4 Alkyl benzene	119(100)134(25)
21	1.40	<1	C_4 Alkyl benzene	105(100)134(15)
22	1.42	<1	C_4 Alkyl benzene	119(100)134(25)
23	[illegible]	1	C_4 Alkyl benzene	119(100)134(30)

TABLE A-34. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 12E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10³
2	880	*	Branched hydrocarbon C ≥ 8	57(100)85(26)41(21)43(20)72(13)	Pentane,2,2-Dimethyl-	490
3	887	*	Alkyl Ketone	85(100)43(92)58(63)45(56)115(22)61(21)	2-Pentanone,3-Methoxy-	305
4	892	*	?	63(100)45(79)85(68)78(11) Poor MS	1,3,5-Trioxane,2,4,6-Trimethyl-	215
5	995	*	?	57(100)105(83)85(80)41(52)120(32)93(23)63(20)		
9	1062	*	Acetophenone	105(100)77(45)43(22)120(15)	Ethanone,1-Phenyl-	460
15	1099	**	Undecane	43(100)57(72)71(41)85(30)156(2)	Undecane	776
18	1136	**	Benzenemethanol,-Ethyl	105(100)107(65)77(58)79(42)134(12)136(4)	Benzene Methanol,Alpha-Ethyl-	450
18a	1136		1-Phenyl 1-Propanone	105(100)77(41)134(12)51(11)	1-Propanone,1-Phenyl-	582
22	1160	*	HC + Naphthalene	128(100)126(32)127(31)		
23	1164	*	Branched Hydrocarbon C ≥ 11	43(100)71(71)57(57)85(50)126(15)	Undecane,2,4-Dimethyl-	631
24	1170	*	Branched Hydrocarbon C ≥ 11	57(100)85(82)71(67)131(55)133(29)	Dodecane,2,5-Dimethyl-	292
26	1182	*	Alkyl Benzene C3	133(100)97(51)119(37)148(36)55(28)56(24)	Benzene,1-Ethyl-3-(1-Methyl Ethyl)-	474
27	1187	*	Branched Hydrocarbon C ≥ 11	43(100)57(71)71(65)85(59)97(56)	Pentadecane,3-Methyl-	487
29	1201	**	Dodecane	43(100)57(62)71(36)85(35)170(2)	Dodecane	810
31	1216	**	Branched Hydrocarbon C ≥ 12	43(100)57(98)71(41)85(22)98(18)112(13)113(12)133(11)	Tridecane,4,8-Dimethyl-	460
32	1223	*	Branched Hydrocarbon C ≥ 12	4.(100)119(86) Poor MS	Tetradecane,1-Chloro	238
36	1240	*	Tetrahydro, Methyl-Naphthalenol	131(100)118(58)146(53)105(38)91(32) Good MS	1,2,3,4-Tetrahydro-6-Methylnaphthalene	441
37	1249	*	Branched Hydrocarbon C ≥ 12	43(100)85(66)57(55)133(21)147(13)	Undecane,2,4-Dimethyl-	309
38	1254	**	Branched Hydrocarbon C ≥ 12	43(100)71(60)85(38)57(37)		
39	1259	*	Branched Hydrocarbon C ≥ 12	44(100)57(49)85(42)71(36)99(18)113(10)141(8)140(7)	Dodecane,2-Methyl	493
40	1265	**	Methyl naphthalene	142(100)141(88)57(67)115(51)85(40)71(36)		
41	1270	*	Branched Hydrocarbon C ≥ 12	43(100)57(90)71(79)84(13)85(10)	Nonane,2-Methyl-	561
43	1279	*		142(100)141(93)115(60)143(13)165(10)	1,4-Methanonaphthalene,1,4-Dihydro-	526
47	1301	**	Tridecane	43(100)57(62)85(37)71(35)184(2)	Undecane,2,6-Dimethyl-	648
54	1349	*	Branched Alkane C ≥ 13	43(100)71(98)83(41)56(37)131(19)147(9)	1-Hexene,3,4,5-Trimethyl-	292
55	1351	*	Branched Hydrocarbon C ≥ 13	43(100)57(91)85(71)71(57)105(34)154(27)	Tetradecane,2,5-Dimethyl-	257
56	1353	*	Branched Hydrocarbon C ≥13	Poor MS		
57	1358	*	Branched Hydrocarbon C ≥ 11	43(100)71(61)57(49)85(43)99(22)145(12)	Heptadecane,2,6,10,14-Tetramethyl-	223
58	1363	**	Branched Hydrocarbon C ≥ 13	43(100)57(52)85(38)71(34)99(18)113(12)155(7)	Tetradecane,4,11-Dimethyl	503
59	1370	*	Branched Hydrocarbon C ≥ 11	43(100)57(99)151(55)85(54)71(48)99(29)	Nonane,2,2,4,4,6,8,8-Heptamethyl-	250

TABLE A-34. (Continued)

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	R.I. x 10^3
60	1376	**	Alkyl naphthalene. C_2	156(100)141(67)155(33)115(30)95(12)157(11)	Naphthalene,1,4-Dimethyl-	258
62	1392	*	Alkyl naphthalene, C_2	156(100)141(83)83(72)88(46)101(41)157(12)		
63	1400	**	Tetradecane	43(100)57(63)85(50)71(45)	Tetradecane	614
72	1463	*	Branched Hydrocarbon C $\geq$ 14	43(100)71(59)57(54)85(49)99(21)113(18)141(16)	Dodecane,2-Methyl-	447
73	1470	*	Branched Hydrocarbon C $\geq$ 14	57(100)43(62)85(61)71(58)99(27)	Tetradecane,2,5-Dimethyl-	453
77	1501	**	Pentadecane	43(100)57(65)85(52)71(52)99(13)170(1)	Dodecane,2,6,11-Trimethyl-	632
82	1598	*	Hexadecane	43(100)57(77)71(62)85(52)99(15)127(7)	Hexadecane	581
84	1680	**	Hexamethylbenzene	Internal Standard		
85	1698	*	Heptadecane	56(100)43(93)71(80)85(61)41(59)		
86	2181	**	Pentadecylbenzene	Internal Standard		

TABLE A-35. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 12E

GC Peak No.	Retention Index	Amount, μg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10^3
4	987	**	Carbitol	65(100)59(33)72(25)104(3)103(2)	Ethanol,2-(2-ethoxy ethoxy)-	563
8	1167	*	2-Hydroxy Benzoic Acid	120(100)92(86)152(4)121(31)65(28)63(22)	Benzoic Acid,2-Hydroxy-Methyl Ester	228
9	1187	*	Benzthiadiazole	135(100)108(41)69(31)82(15)63(13)136(9)91(8)	1,2,3-Benzothiadiazole	373
10	1377	*	?	71(100)43(73)97(17)173(3)172(2)	Butyric Acid, Thio-,S-Decyl Ester	227
11	1509	*	Dodecanoic Acid	74(100)87(61)43(32)55(30)59(20)143(11)171(7)		
12	1554	*	?	181(100)148(86)108(60)69(38)45(39)136(27)180(25)		
13	1709	*	Tetradecanoic Acid	74(100)87(61)43(35)55(29)59(18)143(13)		
14	1885	*	Subst. Fatty Acid C ≥ 15	55(100)74(70)96(44)87(34)181(15) Poor MS		
15	1913	**	Hexadecanoic Acid	Internal Standard		
16	1921	*	Phthalate, Dibutyl	149(100)41(14)76(12)104(11)105(10)150(9)223(2)	1,2-Benzenedicarboxylic Acid,Dibutyl Ester	229
19	1982	*	Subst. Fatty Acid C ≥ 16	74(100)87(63)43(32)55(30)41(27)143(19)185(13)		
22	2073	*	9,12-Octadecadienoic Acid	67(100)81(79)55(61)95(57)41(52)79(51)104(31)	9,12-Octadecadienoic Acid, Methyl Ester	386
23	2083	*	Octadecenoic Acid	55(100)41(68)43(67)69(60)74(52)83(41) [265(1)]?	10-Octadecenoic Acid, Methyl Ester	340
26	2114	*	Octadecanoic Acid	74(100)87(67)43(53)55(37)41(30)143(10)	Heneicosanoic Acid, Methyl Ester	710
27	2121	*	Phenyl subst. Acid	91(100)105(66)77(64)115(62)119(60)252(19)199(10)		
28	2131	*	–	91(100)146(87)153(81)105(82)101(75)41(61)		
29	2139	*	?	146(100)91(55)117(54)133(51)109(33)105(30)		
31	2183	**	Pentadecyl Benzene	Internal Standard		
32	2170	**	Subst. Benzoic Acid	91(100)105(82)79(63)41(64)241(19)302(2)	2,5-Octadecadiynoic Acid, Methyl Ester	375
33	2196	*	?	121(100)91(38)105(32)243(5)244(3)304(2) Good MS		
34	2210	*	?	121(100)91(38)105(32)79(25)55(20)		
37	2248	*	?	43(100)41(63)55(52)261(11)305(3)		
38	2267	*	?	121(100)91(67)79(58)81(54)105(55)107(54)215(17)241(8)257(2)		
39	2275	*	Chloroalkylphenyl Acid	91(100)41(99)43(98)105(85)55(68)79(57)131(54)213(14)243(13)241(12)215(6)		
41	2306	**	Alkyl subst. benzoic acid	43(100)91(78)121(75)105(62)243(22)215(13)304(4)		
45	2355	**	Subt. Benzoic Acid	105(100)91(90)121(80)43(51)185(37)213(31)257(11)256(10)317(4)		
46	2373	*	–	105(100)91(99)131(70)43(60)78(57)146(51)213(15)303(5)		
47	2388	**	?	109(100)43(91)95(88)67(68)91(62)217(35)261(29)305(11)		
55	2487	*	?	43(100)237(78)129(67)41(63)59(60)255(16)		
58	2524	*	?	128(100)59(90)253(83)115(82)187(76)91(52)269(9)		
[illegible]	[illegible]	**		[illegible]		

TABLE A-36. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 13VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.13		Air	44(100)
2	0.16	<1	Dichloromethane	49(100)86(60)
3	0.16	<1	Carbon disulfide	76(100)
4	0.18	10-100	Dichloromethane	49(100)86(60)
5	0.18	~10	Carbon disulfide	76(100)
6	0.24	10-100	Chloroform	83(100)85(70)
7	0.31	10-100	Carbon tetrachloride	117(100)119(95)82(30)
8	0.35	1-10	1,2-Dichloropropane	63(100)62(70)76(40)
9	0.36	1-10	Bromodichloromethane	83(100)85(70)127(10)129(15)
10	0.55	1-10	Toluene	91(100)92(50)
11	1.00	-(8)	I.S.	75(100)110(50)

TABLE A-37. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 14VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.12		Air	44(100)
2	0.13	1-10	Vinyl formate or Acetaldehyde	44(100)43(80)42(25)
3	0.16	1-10	Dichloromethane	49(100)84(90)
4	0.18	<1	Dichloroethylene	61(100)96(40)98,63(30)
5	0.19	<1	2,3-Dimethylbutane	44(100)43(50)42(30)71(20)
6	0.20	<1	3-Methylpentane	57(100)56(95)41(90)71(5)86(4)
7	0.21	<1	N,N-Dimethylformamide (T)	73(100)44(65)45(30)128,130(2)
8	0.21	1-10	Chloroform	83(100)85(70)
9	0.24	<1	Methyl cyclopentane	56(100)41(60)69(40)84(6)
10	0.25	~10	2-Methyl-1,3-dioxolane	73(100)43(90)45(70)58(30)87(10) Big Peak
11	0.35	<1	1,4- Dioxane	88(100)58(93)43(45)
12	0.55	<1	Toluene	91(100)92(50)
13	1.00	-(8)	I.S.	75(100)
14	1.30	<1	Alkane (C_9H_{20})	57(100)43(80)71(40)

TABLE A-38. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 14E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	SI x 10^3
1	856	*	Methylcyclohexane	83(100)55(98)98(50)	Cyclohexane, Methyl-	599
2	861	*	Toluene	92(100)91(98)65(34)	Benzene, -Methyl	569
3	1148	*	N,N-Dimethylacetamide	44(100)87(55)72(20)	Acetamide, N,N-Dimethyl	869
4	1356	***	1,1'-Biphenyl	154(100)153(65)76(55)152(63)51(30)63(25)	1,1'-Biphenyl	630
5	1376	***	Diphenyl Ether	170(100)51(100)77(95)156(92)141(73)	Benzene, 1,1'-Oxybis-	559
6	1677	*	Dibenzofuran	168(100)139(50)89(20)169(18)	Dibenzofuran	455
7	1641	*	1,4-Methanonaphthalen-9-ol, 1,4-Dihydro-	157(100)128(70)129(62)77(31)158(10)	1,4-Methanonaphthalene-9-ol, 1,4-Dihydro-	513
8	1808	*	N,4-Dimethylbenzenesulfonamide	91(100)65(32)185(16)155(18)	Benzenesulfonamide, N,4-Dimethyl	669
9	1920	*	Dibutyl Phthalate	149(100)41(15)150(10)205(3)223(5)	1,2 Benzenedicarboxylic Acid, Butyl 2-	587
					Methylpropyl Ester	

TABLE A-39. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 15VE

GC Peak No.	Relative Retention Time	Amount, μg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.10		Air	44(100)
2	0.10	10-100	Carbonyl sulfide	60(100)62(5)
3	0.13	1-10	Dichloroethylene	61(100)96(70)
4	0.13	10-100	Dichloromethane	84(100)49(95)
5	0.14	10-100	Carbon disulfide (lots)	76(100)44(75)78(35)
6	0.18	10-100	Chloroform	83(100)85(90)
7	0.20	1-10	1,2-Dichloroethane	62(100)49(32)64(30)
8	0.21	1-10	1,1,1-Trichloroethane	97(100)99(70)117,119(20)
9	0.23	1-10	Benzene	78(100)
10	0.23	10-100	Carbon tetrachloride	117(100)119(98)82(30)
11	0.27	10-100	1,2-Dichloropropane	63(100)62(70)76(40)
12	0.27	1-10	3-Pentanone	57(100)86(20)
13	0.28	10-100	Bromodichloromethane	83(100)85(70)127,129,131
14	0.44	1-10	Toluene	91(100)
15	0.48	1-10	Dibromochloromethane	129(100)127(80)208,210
16	0.59	1-10	1,1,2,2-Tetrachloroethene	129(100)166(95)131(90)166(80)
17	1.00	-(8)	I.S.	75(100)
18	1.15	1-10	Butyl ketone (T)	85(100)57(98)100,127(~8)
19	1.17	1-10	Alkane C_8H_{18}	57(100)71,43,85,99

TABLE A-40. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 15E

GC Peak No.	Retention Index	Amount, μg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10^3
1	862	**	OXA Bicyclo [4.1.0] Heptane	83(100)41(72)42(70)54(49)69(35)97(17)98(4)	7-Oxabicyclo [4.1.0] Heptane	578
2	881	**	Cyclohexanol	70(100)83(38)50(37)41(31)97(25)98(20)	2-Cyclohexen-1-ol	608
3	890	**	Chlorocyclohexene	81(100)79(61)80(35)53(27)77(22)	Cyclohexene ,3-Chloro-	612
4	952	*	Dimethylpentanol	57(100)85(70)41(42)58(27)	Pentanol, 2,3-Dimethyl	621
5	1006	**	?	69(100)68(47)41(39)62(26)54(28)	Cyclopentane, Chloro-	319
6	1035	***	Chlorocyclohexanol	57(100)80(25)88(11)90(4)134(3)136(1)	Cyclohexanol, 4-Chloro	520
7	1074	**	?	71(100)41(18)81(13)57(12) poor spectrum		
8	1101	***	Dichlorocyclohexane	81(100)80(56)41(17)88(4)90(3)116(2)118(1)	Cyclohexane, 1,2-Dichloro-, Cis-	595
9	1113	***	Bromocyclohexanol	81(100)57(78)99(23)41(22)132(3)134(3)	Cyclohexanol, 2-Bromo-, Cis-	576
10	1121	**	Bromomethoxycyclohexane	71(100)81(66)41(28)	Cyclohexane, 1-Bromo-2-Methoxy-Cis	638
11	1126	**	Bromochlorocyclohexane	81(100)41(10)53(9)117(8)119(2)	Cyclohexane, 1-Bromo-2-Chloro, Cis-	521
12	1133	**	1-Phenylpropanone	105(100)77(65)51(25)134(12)	1-Propanone, 1-Phenyl	656
13	1140	*	1-Phenylpropanol	77(100)79(82)105(92)107(92)51(41)134(10)136(8)	Benzene Methanol, α-Ethyl-	657
14	1215	*	Dibromocyclohexane	81(100)41(19)161(6)163(6)	Cyclohexane, 1,3-Dibromo-	661
15	1386	*	Hexyloxybutanol	71(100)56(81)43(77)89(53)	1-Butanol, 4-(Hexyloxy)-	613

TABLE A-41. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 16VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.16		Air	
2	0.19	<1	Dichloromethane	49(100)84(50)
3	0.29	<1	1,1,1-Trichloroethane	97(100)61(70)99(60)117,119,116
4	0.39	1-10	Trichloroethylene	95(100)130(80)132(78)97(70)60(60)
5	0.91	1-10	C_2 Alkyl benzene	91(100)106(45)
6	1.00		I.S.	75(100)
7	1.26	1-10	C_3 Alkyl benzene	105(100)120(40)
8	1.43	1-10	C_4 Alkyl benzene	119(100)
9	1.50	1-10	C_4 Alkyl benzene	119(100)

TABLE A-42. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 17VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.11		Air	
2	0.14	<1	Trichlorotrifluoro ethane	101(100)103(70)151(60)153(40)
3	0.15	1-10	Dichloroethylene	96(100)61(80)98(70)59(40)
4	0.15	1-10	Dichloromethane	49(100)
5	0.16	1-10	Trichlorotrifluoroethane	151(100)101(70)153(60)103(50)
6	0.18	1-10	2,3-Dimethylbutane	43(100)42(57)41(65)71(35)
7	0.20	1-10	3-Methylpentane	57(100)56(88)41(70)
8	0.21	10-100	Chloroform	83(100)
9	0.26	<1	Methyl cyclopentane	56(100)41(60)69(60)86(6)
10	0.25	<1	1,1,1-Trichloroethane	97(100)99(70)61(65)117,119,116
11	0.29	<1	Trichloroethylene	95(100)132(90)130(97)
12	0.36	1-10	Toluene	91(100)

TABLE A-43. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 18VI

GC Peak No	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.12	--	Air	44(100)
2	.16	~1	Acetone	43(100)58(30)
3	.16	<1	Diethyl ether	59(100)74(73)45(65)
4	.17	~10	Dichloromethane	49(100)84(40)
5	.23	<1	Chloroform	83(100)85(67)
6	.25	<1	Tetrahydrofuran	42(100)72(32)71(30)
7	.27	<1	1,1,1-Trichloroethane	97(100)61(70)99(65)
8	.29	<1	Benzene	78(100)
9	.36	<1	Trichloroethylene	130(100)95(87)132(75)97(70)
10	.54	<1	Toluene	91(100)92(60)
11	.68	<1	1,1,2,2-Tetrachloroethene	166(100)129(92)164(82)131(70)
12	1.00	-(8)	I.S.	75(100)77(33)

TABLE A-44. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 18VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.14		Air	44(100)
2	0.18	1-10	Dichloroethylene	61(100)96(62)98(40)
3	0.18	10-100	Dichloromethane	49(100)
4	0.25	1-10	3-Methylpentane + Chloroform	41(100)57(92)83(80)43(70)
5	0.29	1-10	1,1,1-Trichloroethane	97(100)99(70)117,119,121
6	0.31	<1	Benzene	78(100)
7	0.57	1-10	Toluene	91(100)
8	1.00	1-10	I.S.	75(100)

TABLE A-45. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 18E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	E.I. x 10^3
1	998	**	Carbitol	45(100)59(35)72(27)104(4)103(1)	Ethane,1,1'-Oxybis[2-Ethoxy-	618
2	1076	**	?	66(100)91(14)87(13)121(5)152(4)		
3	1083	**	?	66(100)91(12)87(10)121(5)122(4)		
4	1233	**	Dimethylhydroxymethoxy benzaldehyde + ?	137(100)83(99)109(51)53(46)180(44)		
5	1261	*	Dichlorobenzoic acid	173(100)175(64)145(39)109(24)74(22)204(20)206(12)207(4)	Benzoic acid,3,4-Dichloro,methyl ester	374
6	1462	**	Indolinecarboxyaldehyde,hydroxy methyl	177(100)163(36)131(32)91(29)178(12)		
7	1506	*	Dodecanoic acid	74(100)87(68)	Dodecanoic acid, methyl ester	318
8	1708	**	Tetradecanoic acid + ?	74(100)87(71)158(83)143(19)211(2)	Tetradecanoic acid, methyl ester	229
9	1769	**	?	140(100)183(76)113(20)63(8)		
10	1779	**	C ≥ 15 Fatty acid	74(100)87(71)143(18)199(14)256(0.1)	Tetradecanoic acid, 12-Methyl-,methyl ester	706
11	1791	**	C ≥ 15 Fatty acid + ?	153(100)152(61)74(30)87(20)212(18)		
12	1836	**	?	198(100)173(32)115(29)129(27)213(21)171(22)76(15)		
13	1886	**	C ≥ 16 Fatty acid	55(100)41(71)74(64)87(44)236(2)	9-Hexadecenoic acid, methyl ester,(z)-	487
14	1910	**	Hexadecanoic acid	71(100)87(72)43(27)55(26)143(19)270(2)	Hexadecanoic acid methyl ester	672
15	1990	*	C ≥ 16 Fatty acid	55(100)69(60)74(55)87(32)157(26)199(15)	13-Octadecenoic acid, methyl ester	321
16	2085	*	C ≥ 18 Fatty acid	55(100)69(65)74(57)87(42)199(17)222(6)	11-Octadecenoic acid, methyl ester	382
17	2111	*	Octadecanoic acid	74(100)87(80)55(28)143(26)255(3)	Heneicosanoic acid,methyl ester	687

TABLE A-46. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 18E

GC Peak No.	Retention Index	Amount, μg^a	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10^3
1	865	**	Methylcyclopentenone	53(100)81(86)67(56)96(54)41(26)95(6)9.7(4)	2-Cyclopenten-1-one, 2-Methyl	700
2	1036	**	Methylpyridine + ?	93(100)66(51)96(10)	Pyridine, 3-Methyl	426
3	1126	**	Naphthalene + ?	128(100)102(20)121(17)127(18)63(10)129(10)		
4	1143	**	Isoquinoline	129(100)102(58)51(40)78(25)130(10)	Isoquinoline	561
5	1193	**	1,6-Naphthridine	130(100)129(26)76(28)103(24)104(23)79(19)50(20)131(9)	1,6-Naphthyridine	683
6	1210	**	1,2-Benzisothiazole C_7H_5NS	135(100)108(20)91(13)82(13)63(12)45(11)136(18)131(9)	1,2-Benzisothiazole	458
7	1239	**	3-Methylcinnoline $C_9H_8N_2$	115(100)116(46)144(44)135(20)63(20)89(15)	Cinnoline, 3-Methyl	396
8	1266	**	Methylnaphthalene + ?	141(100)142(82)115(76)130(70)76(25)103(24)		
9	1271	**	Methylnaphthyridine	144(100)143(42)117(25)145(10)	1,8-Naphthyridine	723
10	1290	***	Methylcinnoline	115(100)144(51)116(42)89(12)63(13)50(10)	Cinnoline, 3-Methyl	525
11	1300	**	Methylisoquinoline $C_{10}H_9N$	143(100)115(76)116(31)63(19)75(16)89(13)144(18)	Isoquinoline, 1-Methyl	478
12	1313	**	Methylcinnoline	115(100)144(54)116(50)89(16)63(14)50(10)145(6)	Cinnoline, 3-Methyl	552
13	1329	*	Dimethylnaphthyridine	158(100)157(36)143(18)130(13)89(9)63(10)159(11)	1,8-Naphthyridine	476
14	1350	**	Mixture ? MW 162	129(100)167(96)115(78)162(68)91(42)77(32)50(28)		
15	1401	**	Pyrrolo[2,3,B]Pyridine Dimethyl $C_9H_{10}N_2$	131(100)145(86)132(78)145(40)63(20)51(18)104(19)118(16)	1H-Pyrrolo[2,3-B] Pyridine, 2-Ethyl	555
16	1427	**	Methylbenzimidazole	131(100)132(80)106(18)77(19)51(16)133(7)	Pyrido[2,3,D]Pyrimidine	382
17	1496	**	Dimethylbenzimidazole + Carbazole	146(100)145(98)167(45)77(27)104(24)131(22)51(20)166(14)168(6)		
18	1530	**	Dimethylbenzimidazole + ? $C_9H_{10}N_2$	146(100)145(68)131(76)118(20)91(20)65(14)160(6)	1H-Benzimidazole, 5,6-Dimethyl	462
19	1540	**	C_3-Benzimidazole + ?	145(100)160(68)159(51)146(67)167(16)91(18)77(16)51(14)		
20	1579	**	Phenanthroline ($C_{12}H_8N_2$)	180(100)153(67)179(26)152(18)126(16)63(10)181(11)		
21	1596	**	Benzo[c]methylcinnoline $C_{13}H_{10}N_2$	165(100)194(97)166(28)195(16)139(12)126(11)63(10)	Benzo[c]cinnoline, 4-Methyl	466
22	1903	*	Mixture ?	168(100)141(30)114(19)140(22)113(12)63(8)169(13)	9H-Pyrido[3,4,B]Indole	399
23	2472	**	?	117(100)131(16)41(16)116(14)203(4)		

TABLE A-47. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 19VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.13	--	Air	44(100)
2	0.16	10-100	Acetone	43(100)
3	0.23	1-10	Chloroform	83(100)
4	0.26	<1	1,1,1-Trichloroethane	97(100)99(70)61(30)117,119,121
5	0.35	<1	Bromodichloromethane	83(100)85(70)127,129,131
6	0.60	<1	Dibromochloromethane	129(100)127(80)131(30)79,81
7	1.00	-(8)	I.S.	75(100)

TABLE A-48. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 20VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.13	--	Air	44(100)
2	0.19	10-100	Dichloromethane	49(100)
3	0.23	1-10	3-Methylpentane	57(100)56(85)41(70)71(5)
4	0.25	10-100	Chloroform	83(100)
5	0.28	<1	Tetrahydrofuran	42(100)41(45)71,72(30)
6	0.29	10-100	Methyl cyclopentane	56(100)69(50)4(42)84(5)
7	0.30	1-10	1,1,1-Trichloroethane	97(100)99(70)61(50)117,119,121
8	0.40	1-10	Bromodichloromethane	83(100)85(70)127,129,131
9	1.00	1-10	I.S.	75(100)
10	1.37	10-100	C_3-Alkyl benzene	105(100)119(80)134(20)
11	1.38	1-10	C_3-Alkyl benzene	105(100)
12	1.39	1-10	C_3 Alkyl benzene	105(100)
13	1.65	10-100	M126 Alkene C_9H_{18}	43(100)55(80)69(60)83,97,111

TABLE A-49. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 21VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.12		Air	44(100)
2	0.16	10-100	Acetone	43(100)58(30)
3	0.17	10-100	Dichloromethane	49(100)
4	0.21	1-10	Methylethyl ketone	43(100)72(20)
5	0.23	1-10	Chloroform	83(100)
6	0.30	1-10	Benzene	78(100)
7	0.50	10-100	4-Methyl-2-pentanone	43(100)58(52)85(15)100(9)
8	0.56	∼10	Toluene	91(100)
9	0.60	10-100	Dibromochloromethane	129(100)127(75)208(9)
10	0.88	1-10	C_2-Alkyl benzene	91(100)
11	1.00	-(8)	I.S.	75(100)

TABLE A-50. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 21E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10^3
1	853	*	Methylpentenal	69(100)41(95)57(73)98(18)	2-Pentenal, 2-Methyl-	365
2	864	***	Hexenal	83(100)54(49)55(45)57(35)60(32)70(22)97(12)98(6)	7-Oxabicyclo[4,1,0] Heptane	616
3	884	**	Cyclohexenol	70(100)83(37)55(35)69(31)41(26)97(25)98(22)	2-Cyclohexen-1-OL	380
4	893	**	Chlorocyclohexene	81(100)79(66)53(24)70(38)116(10)118(4)	Cyclohexene, 3-Chloro-	622
5	912	**	Halo-Alkene	177(100)175(62)61(54)60(36)179(44)212(7)214(5)210(4)178(4)		
6	1015	***	Chlorocyclohexanol	57(100)80*65)44(45)81(41)88(28)98(18)134(10)136(4)	Cyclohexanol, 4-Chloro-, Trans-	501
7	1044	***	Dichlorocyclohexane	80(100)81(99)77(77)55(47)100(49)120(15)152(3)154(2)	Cyclohexane, 1,3-Dichloro-	601
8	1086	***	Bromocyclohexanol	57(100)81(99.5)41(37)99(39)132(5)134(5)178(1)180(1)	Cyclohexanol, 2-Bromo-, Trans-	677
9	1118	**	Bromochlorocyclohexane	81(100)70(36)41(30)53(28)117(20)119(6)	Cyclohexane, 1-Bromo-2-Chloro, Cis-	455

TABLE A-51. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 22VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.16		Air	44(100)
2	0.19	>100	Acetone	43(100)
3	0.20	10-100	Dichloromethane	49(100)
4	0.21	10-100	Carbon disulfide	76(100)
5	0.24	1-10	Methylethyl ketone	43(100)72(20)
6	0.26	1-10	Chloroform	83(100)
7	0.30	1-10	1,1,1-Trichloroethane	97(100)99(70)61(30)112,114(13)
8	0.51	1-10	4-Methyl-2-pentanone	43(100)58(30)85,100
9	0.57	10-100	Toluene	91(100)
10	0.80	1-10	4-Vinyl cyclohexene	54(100)78(80)66(40)91,93(20)
11	0.87	10-100	C_9 Alkene C_9H_{18}	43(100)57(50)71(15)
12	0.87	1-10	C_2-Alkyl benzene	91(100)106(45)
13	1.00	--	I.S.	75(100)
14	1.29	1-10	$C_{10}H_{18}$, e.g., C_4 Alkyl cyclohexene	95(100)67(60)68(38)81(32)41(26)123(21)138(15)

TABLE A-52. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 22E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	RI x 10^3
1	879	**	Toluene	91(100)92(67)65(19)63(12)	Benzene, Methyl	572
2	922	***	Methylhexanone	63(100)59(36)71(10)81(6)114(1)	2-Hexenone, 5-Methyl	807
3	973	**	? + Alkyl-Ketone C ≥ 7	43(100)41(81)69(32)97(34)106(25)78(21)112(18)		
4	1023	**	Methylcyclohexanone	55(100)56(45)41(50)112(23)83(20)	Cycohexanone, 4-Methyl	836
5	1042	**	Methylcyclohexanol	57(100)41(38)58(41)81(40)55(36)70(20)96(13)	Cydohexanol, 4-Methyl	533
6	1050	**	C_3-Alkylbenzene	43(100)77(92)105(82)51(58)120(19)		
7	1061	**	1-Methyl-1-Phenylethanol	63(100)121(38)77(16)51(16)122(4)	Benzene Methanol, α,α-Dimethyl	708
8	1123	**	C_4-Alkylcyclohexanol	71(100)43(74)81(14)98(13)123(7)141(6)	Cyclohexanol, 1-Methyl-4-(1-Methyl Ethyl)-	453
					Trans	
9	1135	**	Alkyl-Alcohol C ≥ 9	59(100)113(10)123(4)	1,8-Nonanediol, 8-Methyl-	496
10	1155	**	C_4-Alkylcyclohexanol	71(100)43(69)72(16)	Cyclohexanol, 1-Methyl-4-(1-Methyl Ethyl)-	471
					Trans-	
11	1166	**	Alkyl-Alcohol C ≥ 9	55(100)41(70)57(43)81(40)83(25)124(17)96(14)109(9)	Cyclohexanol, 4-(1-Methyl Ethyl)-	364
12	1173	**	Alkyl-Alcohol C ≥ 9	55(100)59(86)81(52)95(55)67(47)136(13)	Bicyclo[2,2,1]Heptan-2-ol, 1,7,7,-	515
					Trimethyl-	
13	1299	**	Alkyl-Ketone C > 11	63(100)71(82)59(56)112(10)137(4)155(2)	6,9-Dodecandeione	332
14	1338	**	Alkyl-Alcohol C ≥ 12	63(100)83(81)41(68)69(61)55,56)81(33)97(14)	1,8-Nonanediol	500
15	1654	**	Alkylphenol C ≥ 15	135(100)107(49)91(16)121(12)149(6)	Phenol, 4-(2,2,3,3,tetra methyl butyl)-	475
16	1688	**	Alkylphenol C ≥ 15	121(100)58(76)107(50)163(20)177(7)		
17	1696	**	Nonylphenol C ≥ 15	135(100)107(26)41(16)136(10)	Phenol, 3-(1,1-Dimethyl Ethyl)	445
18	1705	**	Nonylphenol C ≥ 15	107(100)135(67)149(56)121(55)55(22)77(17)91(14)191(10)	Phenol, Nonyl-	656
19	1712	**	Alkylphenol C ≥ 16	107(100)135(96)121(69)91(18)77(19)163(20)177(15)	Phenol, Dodecyl-	621
20	1725	**	Alkylphenol C ≥ 16	107(100)121(68)149(61)77(18)55(18)177(15)		
21	1740	**	Alkylphenol C ≥ 16	135(100)107(44)41(28)121(14)149(12)	Phenol, Nonyl-	532

TABLE A-53. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 22E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	R.I. x 10^3
1	923	**	Phenol	94(100)93(99)92(88)66(99)63(97)50(91) (Saturated)	Phenol	203
2	1062	**	Benzoic acid	136(100)105(100)77(96)51(97) (Saturated)		
3	1162	**	Methylcyclohexene-1-carboxylic acid	80(100)67(96)94(98)122(75)139(9)154(4)	3-Cyclohexene + Carboxylic acid,4-methyl ~~ester~~	349
4	1169	**	Methylcyclohexene-1-carboxylic acid	94(100)95(99)87(99)80(99)67(98)122(82)139(15)154(2)	"	266
5	1506	*	Dodecanoic acid	87(100)74(98)43(76)55(55)143(12)185(2)214(1)		
6	1543	**	?	58(100)41(97)109(80)136(54)168(52)140(38)224(4)		
7	1576	***	C = 14 Branched fatty acid + Nonyl phenol	117(100)59(97)74(98)91(96)131(98)147(99)173(86)220(24)		
8	1599	**	C = 14 Branched fatty acid	132(100)147(98)117(97)91(95)74(54)220(26)205(8)		
9	1695	**	Akylphenol + ?	136(100)137(96)135(85)107(79)220(3)		
10	1703	**	Tetradecanoic acid + Alkylphenol	75(100)87(96)108(97)149(95)136(87)121(78)191(21)220(5)		
11	1727	**	Alkylphenol + ?	108(100)149(96)121(54)55(43)177(26)		
12	1738	**	?	137(100)136(87)43(68)95(33)77(26)91(23)107(20)220(2)		
13	1745	**	Nonylphenol	149(100)135(90)107(86)55(39)77(22)91(16)220(1)	Phenol,nonyl-	558
14	1883	*	Hexadecanoic acid	74(100)69(98)55(94)87(61)236(1)	13-Octadecenoic acid, methyl ester	385
15	1911	**	Hexadecanoic acid	76(100)89(100)56(98)143(60)227(12)270(6)		
16	1990	*	C ≥ 16 Fatty acid	55(100)74(58)87(34)143(2)	15-Octadecanoic acid, methyl ester	547
17	2001	*	C ≥ 16 Fatty acid	74(100)87(99)43(76)55(47)143(11)		
18	2064	***	Octahydrodimethylphenanthrene carboxylic acid	198(100)197(99)131(98)117(87)91(76)257(22)272(14)	Subst. Phenanthrenecarboxylic acid	414
19	2088	**	C ≥ 17 Fatty acid + Isomer of #18	89(100)143(96)129(42)199(20)197(18)255(12)298(10)		
20	2113	**	Mixture ?	146(100)92(99)101(98)133(96)187(39)284(1)316(1)		
21	2137	**	?	92(72)146(65)69(65)104(57)133(46)192(14)284(1)		
22	2158	**	Isomer of 20	146(100)91(64)55(58)123(59)284(1)		
23	2193	**	?	55(80)91(64)146(57)105(38)131(35)241(7)239(5)		
24	2210	**	?	91(53)69(46)115(52)131(54)155(52)157(52)195(24)270(9)		
25	2301	***	Mixture ?	145(100)115(66)241(61)211(58)157(60)171(47)299(2)314(1)		

TABLE A-54. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 22E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	RI x 10^3
1	874	**	Mixture ?	56(100)44(75)112(56)58(24)126(2)	Piperidine,1,2,6-trimethyl	519
2	883	**	Cyanopyridine	104(100)78(74)51(34)77(28)103(51)		
3	918	***	Alkylaziridine + ?	70(100)126(99)41(97)56(82)140(2)		
4	957	***	Methylpyridine	93(100)66(99)65(60)63(18)52(18)41(16)	Pyridine,3-methyl	389
5	1006	**	?	43(100)91(50)55(40)71(35)97(20)126(6)		
6	1009	*	?	86(100)42(44)58(34)111(18)126(3)		
7	1199	**	Alkylamine + ? $C_8H_{19}N$	72(100)44(56)128(10)		
8	1204	**	Mixture ?	44(100)72(67)151(37)107(20)		
9	1216	**	Mixture ?	85(100)70(30)98(23)126(22)154(10)182(4)		
10	1303	**	?	72(100)44(34)115(25)132(16)118(17)175(3)		
11	1337	*	?	43(100)74(72)76(49)85(43)98(33)100(32)173(10)		
12	1353	*	Alkylamine	132(100)115(52)133(37)174(31)77(20)91(19)188(3)	2-Heptanamine, N-(Phenylmethylene)-	423
13	1374	**	N,N-Subst. Formamide	100(100)58(56)72(38)44(30)143(16)200(3)	Formamide, N-Butyl-N-(1-Methyl Ethyl)-	526
14	1393	**	?	72(100)132(80)133(58)77(68)118(44)115(43)186(2)		
15	1441	**	?	43(100)57(72)69(64)112(56)146(22)153(16)209(2)		
16	1461	*	Heptamine, N-(Phenylmethylene)	132(100)105(63)86(50)77(28)146(26)188(31)	2-Heptanamine, N-(Phenylmethylene)	438
17	1506	**	N,N-Subst. Formamide	100(100)58(52)72(37)143(25)44(26)214(3)	Formamide, N-Butyl-N-(1-Methyl Ethyl)-	520
18	1546	**	?	92(98)112(76)69(51)74(43)98(37)144(27)167(10)		
19	1811	*	Alkylamine	44(100)		

TABLE A-55. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 23VI

GC Peak No.	Retention Index	Amount, μg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.15	--	Air	44(100)
2	.16	.1-1	Butadiene	54(100)33(80)35(48)
3	.18	10-100	Dichloromethane	49(100)84,86(100) Sat'd
4	.24	10-100	Chloroform	87(100)85(82)83(58)118(18) Sat'd
5	.29	.76	Benzene	78(100)
6	.35	1-10	Bromodichloromethane	83(100)85(65)129(12)
7	.53	.1-1	Toluene	91(100)92(55)
8	.56	.1-1	C_3H_5Cl	76(100)78(35)
9	.57	.1-1	Dibromochloromethane	129(100)127(80)131(20)
10	.97	.1-1	Ethyl benzene	91(100)106(40)
11	1.00	-(8)	I.S.	
12	1.28	.1-1	C_3 Alkyl benzenes	105(100)120(35)
13	1.50	.1-1	C_4 Alkyl benzene	119(100)134(25)

TABLE A-56. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 23VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.11		Air	44(100)
2	0.16	>100	Acetone	43(100)
3	0.17	1-10	Dichloroethylene	61(100)96(40)
4	0.18	10-100	Dichloromethane	49(100)
5	0.24	1-10	Chloroform	83(100)
6	0.26	1-10	Isopropyl ether	45(100)43(63)87(20)
7	0.27	1-10	1,2-Dichloroethane	62(100)64(30)49(30)98,100
8	0.28	10-100	1,1,1-Trichloroethane	97(100)99(70)61(50)117,119,121
9	0.30	10-100	Benzene	78(100)
10	0.45	1-10	C_8H_{16} -- probably 2,4,4-Trimethyl-1-	57(100)41(50)55(30)97,112
			pentene or diisobutylene	
11	0.50	1-10	C_8H_{16} -- probably 2,3,4-Trimethyl-2-	55(100)97(80)41(38)69(30)112(30)
			pentene	
12	0.55	<1	Toluene	91(100)
13	0.86	<1	C_3-Alkyl cyclohexane C_9H_{18}	55(100)97(35)41(35)69(30)126(10)
14	0.88	1-10	C_2-Alkyl benzene	91(100)106(30)
15	0.91	<1	C_9H_{18} C_3 Alkyl cyclohexane	55(100)41(50)69(40)70(28)91,56,43(18)126(7)
16	0.93	<1	C_3-Alkyl cyclohexane	55(100)41(34)83(125)69(13)126(8)
17	0.94	<1	C_3-Alkyl cyclohexane	55(100)83(50)84(30)41(22)69(20)126(6)
18	0.96	<1	C_3-Alkyl cyclohexane (T)	41(100)69(80)55(69)70(47)104(43)56(38)57(34)111(20)126(12)
19	0.98	<1	C_3-Alkyl cyclohexane (T)	69(100)55(80)41(68)111(50)56(38)70(27)43(22)126(10)
20	1.00	<1	I.S.	75(100)

TABLE A-57. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 23E

GC Peak No.	Retention Index	Amount, μg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	KI x 10^3
1	1164	**	Alkylformamide	72(100)114(47)100(46)58*38)142(18)156(6)	Formamide, N-Butyl-N(1-Methyl Ethyl)	305
2	1192	**	Alkylamine	72(100)106(34)86(28)44(24)55(22)142(19)156(4)	Butylamine, N-Methyl-N-Propyl	313
3	1210	**	Alkylformamide	72(100)59(76)100(48)128(46)114(35)142(18)156(10)170(5)	Formamide,N-Butyl-N-(1- Methyl Ethyl)	290
4	1228	***	Alkylformamide	72(100)86(94)57(75)55(70)114(41)142(31)156(53)128(16)170(12)		
5	1252	***	N,N-Alkyl-Alkylamide	100(100)114(89)156(76)55(70)57(62)86(58)142(52)128(20)170(12)		
6	1311	**	N,N-Alkyl-Alkylamide	142(100)86(82)70(68)55(58)57(52)100(60)156(66)170(14)		
7	1316	**	N,N-Alkyl-Alkylamide	100(100)44(91)128(80)114(74)55(73)70(50)156(34)170(12)		
8	1327	**	N,N-Alkyl-Alkylamide	114(100)100(95)86(76)72(45)142(36)128(30)156(23)170(10)		
9	1331	**	N,N-Alkyl-Alkylamide	128(100)100(96)57(48)70(47)170(7)184(3)		
10	1342	**	N,N-Alkyl-Alkylamide	142(100)50(50)86(33)114(28)100(26)156(13)170(7)		

TABLE A-58. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 24VE

GC Peak No.	Relative Retention Time	Amount, μg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.16		Air	44(100)
2	0.21	1-10	Dichloroethylene	61(100)96(80)98(50)
3	0.21	<10	Dichloromethane	49(100)
4	0.27	<10	Chloroform	83(100)
5	0.31	1-10	1,1,1-Trichloroethane	97(100)99(70)61(45)117,119,121
6	1.00	-(8)	I.S.	75(100)

TABLE A-59. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 25VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.11		Air	44(100)
2	0.14	1-10	Butene or Methyl (C_4H_8) propane	41(100)56(55)
3	0.17	10-100	Acetone	43(100)
4	0.17	1-10	C_5H_{10} + Unknown	41(100)59(80)40(40)55(25)43(15)70(12)78(5)
5	0.18	1-10	Ethanethiol	62(100)47(85)45(52)46(38)61(30)63,64(4)
6	0.18	1-10	Dichloromethane	49(100)
7	0.21	1-10	S-containing Unknown	110(100)95(95)93(90)108(50)112(20)
8	0.24	10-100	Methylethyl sulfide	61(100)76(55)48(52)
9	0.27	1-10	1,2-Dichloroethane	62(100)56(40)64(35)69(20)98,100(3)
10	0.28	<1	1,1,1-Trichloroethane	97(100)61(70)99(60)117,119,121
11	0.31	1-10	2-Pentanone	43(100)86(15)71(4)
12	0.38	1-10	Diethyl sulfide	75(100)47(90)90(70)61,62(60)
13	0.41	1-10	Methyl n-propyl sulfide	61(100)90(50)
14	0.48	10-100	Dimethyl Disulfide	94(100)45(72)79(65)
15	0.57	1-10	3-Methyl-2-thiapentane	75(100)41(80)104(60)56(45)
16	0.62	1-10	Thiacyclopentane	60(100)88(60)41(38)
17	0.65	1-10	Unknown Mixture	142(100)45(95)127(65)94(57)140,147(47)61(37)
18	0.75	1-10	M 108 S-unknown	80(100)108(98)45(50)64(40)
19	0.79	1-10	2-Methyl tetrahydrothiopene	87(100)102(40)
20	0.87	1-10	3-Methyl thiacyclopentane	60(100)102(90)41(68)45(67)74(60)87(50)
21	0.91	1-10	Methyl thiacyclohexane	101(100)67(70)87(65)41(65)116(40)
22	0.94	1-10	Dimethyl thiacyclopentane	101(100)99(52)67(40)116(65)
23	0.95	1-10	Dimethyl thiacyclopentane	101(100)59(50)116(50)
24	0.97	10-100	2,3-Dithiahexane	80(100)122(65)
25	0.99	1-10	Unknown	156(100)128(95)154,126(50)
26	0.99	<1	Methylthiacyclohexane	101(100)116(60) $C_6H_{12}S$ M116
27	1.00	-(8)	I.S.	75(100)
28	1.01	<1	$C_6H_{12}S$	101(100)116(50)41(50)59(40)
29	1.02	<1	$C_6H_{12}S$	101(100)116(40)59(50)41(48)
30	1.06	10-100	$C_4H_{10}S_2$ (1,4-Dithiahexane)	66(100)122(90)94(60)

TABLE A-59. (Continued)

GC Peak No	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
31	1.06	1-10	Methylthiacyclohexane	101(100)116(70)67(50)87(40) $C_6H_{12}S$
32	1.08	1-10	Unknown	61(100)43(90)80(75)45(60)47(28)46(25)84(20)74(10)116(6)130(3)
33	1.11	1-10	Unknown	87(100)116(30)130(5)
34	1.16	1-10	Unknown	128(100)43(78)61(65)126(50)170(30)130(21)124,125(20)12,168(18)
35	1.17	1-10	Unknown	115(100)81(60)101,130(50)59,60,61(31)75(28)
36	1.21	10-100	S-containing Unknown	94(100)66(60)43(55)136(46)61(29)59(15)
37	1.23	1-10	Unknown	101(100)59(33)67(30)130(10)
38	1.25	1-10	Unknown	101(100)130(30)59(30)67(28)
39	1.30	10-100	S-containing Unknown	94(100)136(70)43(65)66(55)61(42)
40	1.32	10-100	Dimethyl dithiahexane	43(100)108(30)61(28)150(10)
41	1.41	1-10	Dimethyl dithiahexane	43(100)108(30)61(25)150(17)
42	1.43	1-10	S-containing Unknown	94(100)61(60)57(35)66(30)150(15)
43	1.62	1-10	1-Methyl-1-(1-thiaethylbenzene) + M 168	138(100)91(90)45(72)123(60)153(50)168(10)
			Unknown	

TABLE A-60. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 25E

GC Peak No	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	KI x 10^3
1	852	**	S-containing ?	80(100)108(81)45(57)64(48)110(7)		
2	868	**	Ethylbenzene	91(100)106(38)105(21)77(21)51(23)	Benzene, 1,2-Dimethyl	549
3	880	**	2,3-Dithiahexane	80(100)43(51)45(38)122(37)64(26)		
4	884	**	Xylene	91(100)106(36)51(22)77(18)65(12)63(11)	Benzene, Ethyl	407
5	903	**	3,4-Dithiahexane	66(100)122(69)96(52)79(11)		
6	952	**	Methyldithiahexane $(C_5H_{12}S_2)$	94(100)43(80)66(65)136(40)59(27)		
7	1035	**	?	Poor Spectra		
8	1042	**	?	67(100)55(69)		
9	1047	**	$C \geq 11$ - Alkene	55(100)83(78)98(15)	2-Pentene, 4,4-Dimethyl	586
10	1156	**	Naphthalene + ?	85(100)128(83)119(64)91(66)59(64)68(60)100(49)		
11	1235	**	C_5-Alkylbenzene	133(100)43(70)79(64)77(54)105(46)51(32)91(25)	Benzene (1 Methyl Butyl)	323
12	1249	**	1H-Inden-1-one, Dihydro	106(100)132(78)78(62)51(38)77(39)74(20)133(9)	1H-Inden-1-one, 2,3-Dihydro	672
13	1263	*	3(2H)-Benzofuranone, Methyl	91(100)119(83)148(79)63(64)77(29)	3(2H)-Benzofuranone, 7-Methyl	555
14	1282	**	C_5-Alkybenzene	133(100)105(62)77(64)148(38)91(25)103(21)119(20)	Benzene, 1-Ethyl-3-(1-Methyl Ethyl)	547
15	1307	**	3(2H) Benzofuranone, Methyl	119(100)148(86)91(70)89(61)63(56)77(41)133(41)	3(2H) - Benzofuranone, 7-Methyl	476
16	1326	**	C_5-Alkenylbenzene	118(100)117(96)91(40)63(40)77(37)146(32)		
17	1347	**	Ethanone, 1-[4-(1-Methylethyl) Phenyl]-	147(100)91(75)63(46)119(63)162(48)78(37)105(12)	Ethanone, 1-[4-(1-Methylethyl) Phenyl]-	528
18	1361	**	1H-Indene, 1-Ethyl-2,3-Dihydro	117(100)146(70)118(52)115(40)91(36)63(33)51(28)89(23)103(16)	1H-Indene, 1-Ethyl-2,3-Dihydro	467
19	1385	**	Alkyl-Alcohol $C \geq 11$	69(100)84(86)70(56)55(46)97(6)91(4)		
20	1600	**	Hexadecane + ?	57(100)70(72)69(68)111(53)95(25)85(17)77(13)		
21	1682	**	$C \geq 16$ Alkane	57(100)71(57)85(34)99(8)115(6)97(6)169(6)	Tridecane, 2-Methyl	586
22	1700	**	Heptadecane + ?	57(100)71(82)85(36)91(23)128(21)168(30)165(27)		
23	1723	**	C_7-1,1'-Biphenyl	153(100)152(75)154(73)182(92)181(21)151(25)76(39)63(38)		
24	1742	**	C_7-1,1'-Biphenyl	153(100)152(62)154(65)151(28)182(75)183(18)	[1,1'-Biphenyl]-4-Carboxaldehyde	603
25	1800	**	Octadecane	57(100)43(89)71(67)85(44)99(12)165(6)	Heptadecane, 2-Methyl	539
26	1907	**	Nonadecane	57(100)43(96)71(62)85(38)99(10)	Pentacosane	644

TABLE A-61. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 26VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	--	--	Air	44(100)
2	0.18	>>>>100	Dichloromethane	49(100)
3	0.19	>100	C_4H_3Cl (?)	86(100)51(85)48(40)47(35)88(15)83(10)
4		>100	C_4H_3Cl (?)	47(100)51(95)86(70)48(55)88(28)83(20)
5	0.30	1-10	Benzene	78(100)
6	0.48	>100	Probably C_7H_{14}, e.g., Tetramethyl	55(100)83(70)41(55)42(40)98(30)
			cyclopropane	
7	0.49	>100	Dimethyl disulfide (2,3-dithiabutane)	94(100)45(70)79(60)41,55(35)
8	0.50	>100	C_6 Ketone + C_6H_{12}	43(100)49(25)58(15)84(15)57(12)85,86(8)41,100(5)
9	0.51	10-100	C_8H_{16}, e.g., Trimethyl cyclopentane	70(100)55(90)41(38)97,112(4)
10	0.55	>>100	Toluene	91(100)
11	0.60	10-100	2,3-Dimethylhexane	43(100)70(45)71(30)41(25)
12	0.60	10-100	Alkane	57(100)43(98)71(12)99(9)114(2)
13	0.62	10-100	Alkane	43(100)57(60)41(40)55(22)70(10)97(9)71,9(5)
14	0.64	10-100	C_8H_{16} Methyl cycloheptane	55(100)97(60)112(20)
15	0.64	10-100	C_8H_{18},e.g., Dimethylhexane	43(100)57(50)41,85(25)
16	0.67	10-100	Hydrocarbon	55(100)83(60)56(60)42,41(58)
17	0.68	10-100	Alkene M112	55(100)41(58)56(55)83(47)70(40)42(35)69(30)97,112(12)
18	0.70	10-100	Alkene M112	55(100)97(65)41(48)56(33)42(32)69(27)112(20)70(18)
19	0.73	10-100	Hydrocarbon	43(100)41(60)57(30)85(22)55,56(20)42(19)71(15)97(5)114(3)
20	0.75	>100	Alkane	43(100)41(35)57(28)85(22)71(15)114(2)
21	0.85	>100	Hydrocarbon	55(100)83(90)41(72)43,82(47)56(22)42(20)67,69,112(18)
22	0.88	>100	Hydrocarbon	43(100)41(45)57(40)42,69,71(25)111(122)56,55(20)85(10) Sm 113,1-128
23	0.90	>100	Hydrocarbon + C_2 alkyl benzene	57(100)43(55)41(50)91(45)55(40)56(28)71(18)70(15)
24	0.91	>100	C_2 Alkyl benzene	91(100)106(25)
25	0.93	>100	C_2 Alkyl benzene	91(100)106(30)
26	0.97	>100	C_2 Alkyl benzene	91(100)106(38)
27	1.00	>100	Hydrocarbon	43(100)41(35)57(22)71(16)55,85(15)70(12)
28	1.01	>100	Hydrocarbon	41(100)57(70)62,69(55)56(52)43,55(48)111(23)40(18)126(8)
29	1.05	[illegible]	[illegible] Alkyl benzene	91(100)

TABLE A-61. (Continued)

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
30	1.05	>100	Hydrocarbon	57(100)41(20)83(10)75(5)110(2)
31	1.06	>100	Hydrocarbon	55(100)97(50)41(45)69(26)56(23)126(5)
32	1.12	>100	C_9 Alkane	43(100)57(65)41(40)42,56,85(18)40,71,55(10)99(2)128(1)
33	1.14	>100	C_3-Alkyl benzene	105(100)120(20)
34	1.22	>100	C_3-Alkyl benzene	91(100)120(20)
35	1.25	>100	C_3-Alkyl benzene	105(100)120(20)
36	1.28	>100	C_3-Alkyl benzene	120(100)105(80)
37	1.30	>100	C_3-Alkyl benzene	105(100)
38	1.35	>100	Unknown	120(100)119(30)
39	1.37	10-100	C_4-Alkyl benzene	105(100)77,79(15)134(1)
40	1.40	>100	C_3-Alkyl benzene	105(100)120(30)
41	1.41	>100	C_4-Alkyl benzene	119(100)91(30)134(15)
42	1.42	>100	C_9H_{10}, e.g., Methyl styrene	117(100)118(50)115(30)
43	1.44	10-100	Substituted cyclohexane	55(100)83(78)43(75)71(62)82(55)
44	1.47	>100	C_4-Alkyl benzene	105(100)119(45)134(20)
45	1.50	>100	Unknown	105(100)77(15)
46	1.56	>100	Unknown hydrocarbon	55(100)97(62)41(24)96(12)111(5)
47	1.57	>100	C_4 + C_5-Alkyl benzene	119(100)105(80)91(40)134(20)133(13)148(8)
48	1.60	>100	Alkane	43(100)57(90)71(35)85(20)
49	1.63	>100	$C_{10}H_{12}$ (ethyl styrene)	117(100)115,132(23)
50	1.65	10-100	C_5-Alkyl benzene	105(100)148(2)
51	1.67	10-100	C_5-Alkyl benzene	119(100)91,133,148(13)
52	1.69	10-100	Naphthalene	128(100)

TABLE A-62. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 26E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	SI x 10^3
1	871	***	Butylacetate	43(100)51(30)61(15)73(14)61(14)	Acetic Acid, Butyl Ester	685
2	881	**	Ethylbenzene	91(100)105(25)77(13)65(12)51(12)	Benzene, Ethyl	520
3	888	**	Xylene	91(100)106(37)77(15)51(16)65(11)	Benzene, Ethyl	613
4	900	***	Xylene	91(100)106(37)105(15)77(14)51(13)65(12)	Benzene, 1,4-Dimethyl	470
5	906	**	2-Butoxyethanol	57(100)45(68)41(43)87(18)75(9)	Ethanol, 2-Butoxy	802
6	938	**	C$_3$-Alkylbenzene	91(100)65(21)120(18)51(15)77(10)	Benzene, propyl-	403
7	966	**	C$_3$-Alkylbenzene	105(100)120(26)77(21)91(18)51(13)65(11)	Benzene, 1-Ethyl-2-Methyl	636
8	955	**	C$_3$-Alkylbenzene	105(100)120(40)77(17)91(13)51(10)65(8)	Benzene, 1-Ethyl-2-Methyl	593
9	965	**	C$_3$-Alkylbenzene	105(100)120(25)77(20)79(18)91(18)51(15)	Benzene, 1-Ethyl-2-Methyl	617
10	981	***	C$_3$-Alkylbenzene	105(100)120(35)77(18)91(13)51(11)65(8)	Benzene, 1-Ethyl-2-Methyl	678
11	1003	**	Decane	57(100)43(99.5)41(70)71(38)85(30)	Hexane 3,3-Dimethyl	575
12	1006	***	C$_3$-Alkylbenzene	105(100)120(35)77(15)91*12)51(10)63(7)	Benzene, 1-Ethyl-2-Methyl	633
13	1016	**	Methylstyrene	117(100)118(60)115(34)91(25)63(18)51(12)	Benzene, 1- Ethenyl-3-Methyl	550
14	1021	**	Ethylhexanol	57(100)41(55)55(38)70(21)83(18)117(12)	1-Hexanol, 2-Ethyl-	610
15	1035	***	C$_4$-Alkylbenzene	105(100)119(92)91(38)134(37)77(26)51(15)	Benzene, 1,2-Diethyl	695
16	1041	***	C$_4$-Alkylbenzene	105(100)134(24)77(19)91(15)51(10)119(11)	Benzene (1-Methylpropyl)	637
17	1045	***	C$_4$-Alkylbenzene	105(100)119(64)91(50)134(32)77(25)51(15)65(12)	Benzene, 1,2-Diethyl	743
18	1051	**	C$_4$-Alkylbenzene	119(100)134(24)91(20)77(18)51(11)	Benzene, 2-Ethyl-1,4-Dimethyl	623
19	1055	**	C$_4$-Alkylbenzene	105(100)134(18)77(19)91(12)51(11)	Benzene (1-Methylpropyl)-	511
20	1062	***	C$_4$-Alkylbenzene	119(100)91(30)134(29)77(17)51(10)65(9)	Benzene, 2-Ethyl-1,4-Dimethyl	636
21	1068	***	C$_4$-Alkylbenzene	119(100)91(26)134(24)77(13)41(12)57(11)105(11)	Benzene, 2-Ethyl-1,4-Dimethyl	606
22	1087	***	C$_5$-Alkylbenzene	119(100)91(34)134(24)105(21)77(18)51(12)65(11)145(4)	Benzene, (1,1-Dimethylpropyl)	470
23	1106	***	HC + C$_6$-Alkylbenzene	57(100)43(95)71(44)85(21)119(25)134(12)168(1)	Benzene, 1,2,3,5-Tetramethyl	542
24	1118	***	C$_4$-Alkylbenzene	119(100)134(38)91(22)77(12)65(7)	Benzene, 1,2,4,5-Tetramethyl	671
25	1127	***	Ethylstyrene + HC	117(100)132(33)91(23)77(13)63(11)148(3)	Benzene, 1-Ethenyl-4-Ethyl	502
26	1133	***	C$_5$-Alkylbenzene	117(100)119(55)91(34)115(35)132(30)148(11)	Benzene (1-Ethylpropyl)	447
27	1136	**	C$_4$-Alkylbenzene	119(100)134(34)91(25)77(14)51(11)	Benzene (1,2,3,5-Tetramethyl)	666
28	1157	***	Naphthalene	128(100)73(19)51(13)63(11)102(15)119(13)148(2)	Naphthalene	258
29	1184	**	C$_5$-Alkylbenzene	133(100)148(25)91(22)105(17)77(15)51(11)	Benzene, 1-Ethyl-2,4,5-Trimethyl-	580
30	1193	**	C$_5$-Alkylbenzene	133(100)148(27)91(30)105(21)77(18)51(12)	Benzene, 1-Ethyl-3-(1-Methylethyl)	[illegible]

TABLE A-62. (Continued)

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10^3
31	1203	**	Dodecane	57(100)43(89)41(65)71(54)85(28)98(5)99(5)	Dodecane	767
32	1244	**	Methylnaphthalene	142(100)141(88)115(60)43(23)63(20)143(10)	Naphthalene, 2-Methyl	272
33	1335	***	C $\geq$ 13 Alkene	71(100)43(92)41(43)56(35)55(33)83(26)173(3)	1-Hexene, 3,4,5-Trimethyl	356
34	1355	***	Alkyl-Alcohol C $\geq$ 12	71(100)43(93)56(74)89(55)156(13)173(6)	1-Butanol, 4-(Hexyloxy)-	502
35	1515	**	Trichloro - ?	247(100)245(78)203(30)202(40)249(48)251(10)		
36	1943	**	Trichloro - ?	118(100)47(69)63(67)264(41)262(32)267(20)279(35)277(26)281(17)		
37	1966	**	C $\geq$ 19 Alkane	57(100)43(95)71(64)85(41)127(5)	Tetracontane	663
38	1999	***	Trichloro - ?	79(100)118(60)63(46)245(20)293(15)297(10)299(12)		
39	2101	**	Heneicosane	57(100)43(89)71(65)85(41)99(12)113(7)155(2)	Pentacosane	766
40	2202	**	Docosane	57(100)43(88)71(67)85(44)99(14)113(8)127(6)141(4)	Pentacosane	813
41	2306	**	Tricosane	57(100)43(85)71(68)85(44)99(14)113(9)127(6)	Tetracontane	770
42	2291	**	Butylbenzyl-Phthalate	149(100)91(90)65(27)104(20)123(12)206(11)	1,2-Benzenedicarboxylic Acid, Butyl 2-Methylpropyl Ester	349
43	2405	**	Tetracosane	57(100)43(82)71(69)85(47)99(18)113(11)155(4)	Tetracontane	733
44	2509	**	Pentacosane	57(100)43(82)71(68)85(45)99(15)113(10)127(6)141(5)183(1)	Pentacosane	728
45	2551	**	C $\geq$ 25 Alkane	57(100)43(82)71(67)85(44)113(10)183(1)	Docosane, 11-Decyl-	756
46	2605	**	Hexacosane	57(100)43(78)71(68)85(46)99(16)113(10)183(2)	Docosane, 11-Decyl-	707
47	2696	**	Heptacosane	57(100)43(80)71(67)85(44)99(16)113(10)127(7)	Tetracontane	663
48	2803	**	Octacosane	57(100)43(84)71(64)99(14)113(9)155(2)	Tetracontane 3,5,24-Trimethyl	687
49	2905	**	Nonacosane	57(100)43(83)71(61)85(40)99(15)113(10)127(6)	Tetracontane 3,5,24-Trimethyl	571

TABLE A-63. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 26E

GC Peak No	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10^3
1	895	**	2-Butoxy ethanol	57(100)45(83)41(68)87(26)75(12)100(2)	Ethanol,2-Butoxy	750
2	906	**	Hexanoic acid	74(100)43(99)59(61)87(56)55(39)99(26)101(11)	Butanoic acid, methyl ester	523
3	1004	**	Heptanoic acid	74(100)43(44)87(30)59(18)101(10)113(9)	Heptanoic acid, methyl ester	452
4	1027	***	C ≥ 8 Fatty acid	57(100)87(99)102(99)59(43)69(25)115(20)130(16)	Hexanoic acid, 2-ethyl, methyl ester	627
5	1061	**	Benzoic acid	105(100)77(66)136(25)51(26)119(18)	Benzoic acid, methyl ester	517
6	1103	**	Octanoic acid	74(100)43(53)87(40)55(28)57(23)59(22)127(5)	Octanoic acid, methyl ester	636
7	1146	**	Methylbenzoic acid	91(100)119(96)118(69)65(40)90(28)150(28)	Benzoic acid, 2-methyl, methyl ester	603
8	1203	**	Nonanoic acid	74(100)87(59)43(46)55(28)59(19)141(6)143(5)	Nonanoic acid, methyl ester	691
9	1274	**	Decanoic acid	74(100)87(48)43(26)55(18)59(12)143(8)155(4)157(1)	Decanoic acid, methyl ester	758
10	1340	**	Trimethylbenzoic acid	146(100)147(77)119(79)91(70)131(60)77(48)103(42)178(33)	Benzoic acid,2,4,5-Trimethyl methyl ester	526
11	1355	**	Trimethylbenzoic acid	147(100)91(47)119(42)77(24)178(26)	Benzoic acid,2,4,5-Trimethyl, methyl ester	722
12	1391	**	?	103(100)43(67)71(43)74(40)61(24)163(2)		
13	1505	*	Dodecanoic acid	74(100)87(56)143(8)171(3)214(1)	Dodecanoic acid, methyl ester	716
14	1517	***	Trichloro + ?	247(100)245(80)249(47)251(10)		
15	1672	**	Benzenesulfonamide N,4-Dimethyl	91(100)65(28)155(12)185(7)121(6)	Benzenesulfonamide,N,4-Dimethyl	614
16	1706	**	Tetradecanoic acid	74(100)87(55)143(8)199(2)	Tetradecanoic acid, methyl ester	818
17	1911	**	Hexadecanoic acid	87(100)74(99)43(90)55(61)143(17)270(2)	Hexadecanoic acid, methyl ester	549
18	1980	**	C ≥ 14 Fatty acid	74(100)87(62)143(12)199(2)241(2)	Cyclopentanetridecanoic acid, methyl ester	646
19	2007	*	C ≥ 15 Fatty acid	74(100)87(60)143(8)199(2)	Heneicosanoic acid, methyl ester	649
20	2049	**	C ≥ 17 Fatty acid	67(100)81(73)41(58)55(47)95(32)109(25)	9,12,15-Octadecatrienoic acid, methyl ester,(z,z,z)	491
21	2073	***	Octadecadienoic acid	67(100)81(75)55(69)41(66)95(45)109(18)197(4)	12,15-Octadecadienoic acid, methyl ester	688
22	2085	***	Octadecenoic acid	55(100)69(86)74(79)87(47)143(2)264(3)	10-Octadecenoic acid, methyl ester	743
23	2113	**	Octadecanoic acid	87(100)74(99)43(74)55(49)143(17)199(4)298(1)	Heptadecanoic acid,15-methyl, methyl ester	605
24	2120	**	Octadecadienoic acid	67(100)81(70)95(50)299(3)	12,15-Octadecadienoic acid, methyl ester	734
25	2163	**	Octadecadienoic acid	67(100)81(64)41(47)55(44)95(38)109(15)294(0.5)	12,15-Octadecadienoic acid, methyl ester	677
26	2249	**	C ≥ 18 Fatty acid	67(100)81(73)41(88)55(88)	9,12,15-Octadecatrienoic acid, methyl ester	482
27	2298	**	C ≥ 18 Fatty acid	55(100)87(70)74(45)	Octadecanoic acid, 12-hydroxy, methyl ester	476

TABLE A-64. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 27VE

GC Peak No.	Relative Retention Time	Amount, μg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.10	--	Air	44(100)
2	0.14	>100	Acetone	43(100)58(70)
3	0.21	>>>100	Isopropyl alcohol	45(100)43(20)59(2)
4	1.00	-(8)	I.S.	75(100)

TABLE A-65. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 28VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.14		Air	44(100)
2	.15	10-100	Butene tacetaldehyde (T)	44(100)43(58)41(48)56(32)42(22)
3	.17	>>100	Acetone	43(100)
4	.19	>100	Dichloromethane	49(100)
5	.20	>100	Isobutyraldehyde	43(100)41(60)72(40)
6	.21	1-10	2-Methylpropenal (methacidein)	41(100)70(70)42(30)41(25)
7	.23	10-100	Methyl ethyl Ketone	43(100)72(18)
8	.25	1-10	Chloroform + C_7 Hydrocarbon	41(100)43(96)57(95)83(90)85(60)
9	.30	1-10	1,1,1-Trichloroethane	97(100)61(70)99(60)117,119,121
10	.36	1-10	Tetramethylcyclopropane (T)	55(100)83(60)41(60)98(20)
11	.49	1-10	n-Heptane	43(100)57(28)85(10)100(5)
12	.56	>100	Toluene	91(100)92(60)
13	.62	10-100	Ethyl methyl-1,3-dioxolane	87(100)59(90)41(50)72(20)110(5)
14	.89	>100	Unknown	106(100)65(60)51(50)
15	.66	>100	C_7 Ketone	43(100)71(20)87(5)114(5)
16	.86	1-10	Unknown	87(100)59(80)41(60)56,43(38)129(2)
17	.87	>100	C_2 Alkyl benzene	91(100)106(30)
18	.97	>100	Cyclooctatetraene	104(100)78(60)51(32)
19	.98	>100	C_2 Alkyl benzene	91(100)106(50)
20	1.05	1-10	Unknown	43(100)71(75)41(52)56(40)89(12)101(2)
21	1.05	1-10	C_3 Alkyl benzene	105(100)120(20)
22	1.12	1-10	C_3 Alkyl benzene	91(100)120(20)
23	1.15	10-100	C_3 Alkyl benzene	105(100)120(20)
24	1.15	10-100	C_3 Alkyl benzene	105(100)120(22)
25	1.17	10-100	C_3 Alkyl benzene	105(100)120(35)
26	1.18	10-100	C_9H_{10} Methyl styrene	118(100)117(95)103(60)78(50)
27	1.20	>100	Unknown	55(100)69(95)115(90)41(80)45(46)43(42)71(20)157(3)
28	1.22	10-100	C_3 Alkyl benzene	105(100)120(38)
29	1.25	>100	Hydrocarbon	57(100)56(73)41(65)72(40)
30	1.28	10-100	C_3 Alkyl benzene	105(100)120(35)

TABLE A-65. (Continued)

GC Peak No.	Relative Retention Time	Amount µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
31	1.30	1-10	C_9H_{10}-eg Methyl styrene	117(100)118(68)115(38)63(18)91(12)
32	1.33	10-100	C_4- Alkyl benzene	105(100)119(75)134(25)
33	1.34	1-10	C_4- Alkyl benzene	105(100)134(17)
34	1.35	10-100	C_4 Alkyl benzene	105(100)119(50)91(60)134(28)
35	1.35	10-100	C_4- Alkyl benzene	119(100)91(30)134(18)
36	1.37	1-10	C_4- Alkyl benzene	105(100)134(5)
37	1.39	10-100	C_4 Alkyl benzene	119(100)91(28)134(20)
38	1.39	10-100	C_4 Alkyl benzene	119(100)134(15)
39	1.41	10-100	C_4 Alkyl benzene	119(100)91(30)134(20)
40	1.41	1-10	C_4 Alkyl benzene + alkane	119(100)134(20)
41	1.44	1-10	C_4 + C_5- Alkyl benzene	119(100)105(67)91(60)134(12)148(3)
42	1.46	1-10	C_4- Alkyl benzene	119(100)134(20)
43	1.47	10-100	C_4 Alkyl benzene	119(100)134(28)91(22)
44	1.49	1-10	C_2-Styrene	117(100)115(30)132(25)
45	1.50	1-10	C_5 Alkyl benzene	119(100)91(29)148(12)
46	1.51	1-10	C_2- Alkyl styrene + C_5- Alkyl benzene	117(100)115(27)132,133(20)148(5)
47	1.52	1-10	C_5- Alkyl benzene	119(100)91(30)148(9)
48	1.52	1-10	C_4 Alkyl benzene	119(100)134(30)
49	1.52	1-10	Unknown	105(100)106(82)104(75)91(60)132,148(12)
50	1.56	1-10	Naphthalene	128(100)
51	1.61	1-10	C_5 Alkyl benzene	133(100)105(30)91(29)148(20)
52	1.64	1-10	Alkane	43(100)57(95)71(65)85(20)
53	1.92	>100	Biphenyl	154(100)153(40)77(38)
54	1.97	>100	Diphenyl ether	51(100)77(95)170(90)141(70)142(65)115(60)

TABLE A-66. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 28E

GC Peak No.	Retention Index	Amount, μg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	RI x 10³
1	853	**	Dimethyl-3-Pentanone	43(100)71(90)41(42)70(20)114(16)87(5)	3-Pentanone, 2,4-Dimethyl	516
2	866	***	Ethylbenzene	91(100)106(25)51(13)65(11)77(8)	Benzene, Ethyl-	769
3	878	***	O-Xylene	91(100)106(68)51(31)65(26)77(26)	Benzene, 1,4-Dimethyl	536
4	890	***	P-Xylene	91(100)106(88)77(38)105(38)51(36)	Benzene, 1,4-Dimethyl	629
5	903	**	2-Butoxyethanol	57(100)45(50)41(44)61(25)87(18)75(10)		
6	928	**	Propanoic Acid, 2-Methylpropyl Ester	71(100)43(81)41(57)57(51)89(23)91(8)106(3)	Propanoic Acid, 2-Methylpropyl Ester	581
7	962	**	C_3-Alkylbenzene + ?	56(100)41(60)105(57)69(51)57(43)115(33)120(12)		
8	964	***	Mixture ?	56(100)69(96)115(86)71(26)73(12)157(4)		
9	976	**	C_3-Alkylbenzene	105(100)120(33)77(20)91(15)51(15)121(2)	Benzene, 1,2,4-Trimethyl-	664
10	1002	**	Decane			
11	1099	**	Undecane			
12	1355	***	1,1'-Biphenyl	154(100)153(41)152(31)76(25)51(17)63(13)	1,1'-Biphenyl	500
13	1389	***	Diphenyl Ether	51(100)77(97)141(49)170(50)	Benzene, 1,1'-Oxybis-	461

TABLE A-67. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 28E

GC Peak No.	Retention Index	Amount, μg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	RI x 10³
1	907	**	C ≥ 6 Fatty acid	74(100)43(58)59 (34)87(33)99(16)101(8)	Pentanoic acid,3-methyl, methyl ester	560
2	987	**	Carbitol	45(100)59(42)72(23)43(22)89(2)103(2)104(1.7)	Ethane,1,1'-Oxybis[2-ethoxy-	595
3	999	***	Phenol	94(100)66(71)40(21)95(7)	Phenol	557
4	1063	**	Benzoic acid	105(100)77(67)51(61)136(28)106(8)	Benzoic acid, methyl ester	603
5	1105	**	Octanoic acid	74(100)41(61)55(32)87(40)127(7)	Octanoic acid, methyl ester	470
6	1363	**	Diphenyl ether	170(100)141(89)51(83)77(64)115(36)169(25)	Benzene,1,1'-Oxybis-	597
7	1506	**	Undecanoic acid	74(100)41(56)67(56)55(38)115(8)170(7)183(1)	Cyclopentaneundecanoic acid, methyl ester	489
8	2070	**	Octadecadienoic acid	67(100)41(90)55(80)81(69)95(40)109(16)197(6)	9,11-Octadecadienoic acid, methyl ester	609
9	2080	**	Octadecenoic acid	41(100)55(99.5)69(50)74(46)87(26)180(2)	10-Undecenoic acid, methyl ester	516
10	2165	**	C ≥ 18 Fatty acid	74(100)87(70)43(50)41(38)55(36)143(16)199(6)	Heneicosanoic acid, methyl ester	859
11	2298	**	C_3-Alkyl,octahydro,phenanthrene carboxylic acid	43(100)141(65)55(61)59(50)239(80)299(10)314(4)	1-Phenanthrene carboxylic Acid, ethyl-7-(1-Methyl ethyl)-Methyl Ester	665

TABLE A-68. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 29VE

GC Peak No.	Relative Retention Time	Amount ng	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.17	—	Air	44(100)
2	0.18	1-10	Dimethyl sulfide (B)	62(100)47(87)45(68)46(35)61(30)74(10)108,110(2)
3	0.18	1-10	Dichloromethane	49(100)
4	0.20	<1	1,1-Dichloroethane +	65(100)63(80)43(30)45(28)98(6)100(3)
	Combined	1-10	Ethyl isopropyl ether (T)	
5	0.23	1-10	Hexene (T)	56(100)41(80)55(70)
6	0.26	1-10	Chloroform	83(100)
7	0.27	10-100	Dichloroethane	62(100)64(75)49(72)
8	0.29		Dichloroethane	49(100)64(100)62(85)63(45)98,100
9	0.31	1-10	Benzene	78(100)
10	0.48	<1	Dimethyl disulfide	94(100)46(70)79(60)46(38)
11	0.53	<1	1,1,2-Trichloroethane (B)	97(100)83(92)61(70)99(60)85(60)132,134(5)136(3)
12	0.55	1-10	Toluene	91(100)92(50)
13	0.62	1-10	1,1-Dibromoethane	107(100)109(90)
14	0.69	10-100	Octene	43(100)55(78)70(60)83(20)112(4)
15	0.72	<1	Octane	43(100)41(40)56(30)85(25)71(15) Sm 114
16	0.74	<1	2-Octene M 112	55(100)41(70)70(38)112(30)
17	0.76	<1	S-containing Unknown	80(100)108(95)45(45)64(40)
18	0.77	<1	C_8H_{16} (octene or trimethyl cyclopentane)	55(100)41(80(56(60)70(45)112(30)
19	0.98	1-10	Dimethyl hexene (T)	55(100)41(28)69(22)83(20)126(12)97(10)
20	1.00	~ 8	I S	75(100)
21	1.05	1-10	Ethyl-1-methyl ethyl disulfide $C_5H_{12}S_2$	66(100)122(80)94(55)
22	1.06	<1	Nonone M128	43(100)57(85)85(30)
23	1.24	<1	$C_{10}H_{20}$ eg Methyl nonene	55(100)56(65)69(58)43(50)41(45)58(30)70(20)83(18)140(3)
24	1.25	<1	Unknown	41(100)43(58)69(50)
25	1.27	1-10	$C_{10}H_{20}$ eg 5-Methyl-4-nonene	55(100)69(70)56(50)41(40)83(20)70(19)140(8)
26	1.29	10-100	1-Decene	56(100)55(92)41(85)43(70)70(65)69(55)57(54)83(30)
27	1.30	1-10	$C_{10}H_{20}$ eg Dimethyl octene	43(100)55(85)41(86)69(72)56(62)70(45)71(62)7(12)111(5)140(5)
28	1.31	1-10	Decane	43(100)57(82)41(32)71(27)85(12)56(12)
29	1.32	1-10	Hydrocarbon	55(100)41,43(65)56(60)69(55)70(50)83(11)97,111(10)140(5)

TABLE A-68. (Continued)

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
30	1.33	1-10	hydrocarbon	55(100)43(95)56(85)41(62)69(60)70(40)42(30)83,97(10)140(5)
31	1.51	1-10	Undecane	43(100)57(90)71(43)85(20)
32	1.58	1-10	C_9 Ketone (T)	71(100)43(65)99(20)55(10)
33	1.60	1-10	naphthalene	128(100)

TABLE A-69. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 29E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	RI x 10³
1	856	**	Toluene	91(100)92(58)65(18)51(11)	Benzene, Methyl	563
2	875	**	Octanol	55(100)41(95)43(80)70(58)83(20)112(5)	1-Octanol	680
3	972	**	Methyloctene	56(100)43(62)41(61)69(30)84(5)91(3)	1-Octene, 2-Methyl	572
4	989	***	Decene	41(100)55(95)70(70)83(73)97(13)111(6)140(2)	1-Decene	867
5	1003	***	Propylheptanol	43(100)41(82)57(78)55(71)70(36)85(15)97(6)140(8)162(1)	1-Heptanol, 2-Propyl	520
6	1016	**	Decene	55(100)41(96)56(78)69(56)97(11)140(12)	1-Decene	807
7	1156	**	Dimethyldecene	56(100)41(53)69(60)128(13)111(9)168(2)	1-Octene, 7-Methyl	714
8	1163	***	Dimethyldecene	56(100)55(92)41(89)69(60)83(11)111(9)168(2)	3-Heptene, 2,6-Dimethyl	696
9	1202	***	Dodecene	55(100)41(95)70(80)83(68)57(28)168(0.5)	1-Dodecene	807
10	1215	**	Undecene	55(100)41(70)69(65)83(37)153(20)168(16)170(2)	1-Undecene	550
11	1230	**	Methoxy-C_3-Benzene	135(100)91(98)121(42)150(33)77(30)	Benzene, 2-Methoxy-1,3,5-Trimethyl	516
12	1297	**	C_4-N,N-Subst.-Aniline	134(100)57(44)63(39)71(28)119(28)149(31)		
13	1302	**	Isomer of 12	139(100)149(30)120(27)91(20)77(16)		
14	1356	***	1,1'-Biphenyl	154(100)153(42)152(30)76(24)56(22)155(16)	1,1'-Biphenyl	639
15	1376	***	Diphenyl Ether + ?	170(100)51(95)77(88)141(91)142(81)169(28)171(13)	Benzene, 1,1'-Oxybis-	568
16	1385	***	? + 15	Mixed Spectra		
17	1395	***	Tetradecane	57(100)43(76)71(58)85(30)97(11)111(4)196(1)198(0.3)	Tetradecane	497
18	1405	***	Tetradecene	55(100)41(79)69(56)83(34)97(25)111(9)196(1)	1-Tetradecene	810
19	1416	**	C ≥ 14 Alkane	43(100)57(96)71(70)55(55)85(34)168(1.9)167(1.8)		
20	1467	**	C ≥ 15 Alkane	57(100)43(90)71(76)41(58)85(35)99(8)139(6)168(8)	Pentadecane	735
21	1502	**	Pentadecane	Same as Above		
22	1560	**	C ≥ 15 Alkene	55(100)60(81)41(69)83(61)97(20)111(21)224(1)	6-Tridecene, 7-Methyl-	782
23	1560	***	C ≥ 15 Alkene	56(100)69(69)41(42)83(25)111(15)224(0.4)	6-Tridecene, 7-Methyl-	778
24	1566	**	C ≥ 15 Alkene	56(100)41(36)57(36)69(32)70(32)83(12)97(8)156(1)	1-Pentadecene	691
25	1591	***	Hexadecene	70(100)55(86)41(65)83(60)97(25)111(11)125(6)	1-Hexadecene	828
26	1604	***	Hexadecane	57(100)43(75)71(63)55(58)41(55)85(30)	Heneicosane	577
27	1615	**	Hexadecene	55(100)41(78)69(50)83(46)97(30)111(17)125(5)224(1)	1-Hexadecene	872
28	1666	**	Hexadecene	55(100)41(96)43(82)57(59)69(69)83(55)97(35)111(16)168(1)	1-Hexadecene	792
29	1702	**	Heptadecane	57(100)43(90)41(60)71(79)55(35)85(35)182(1.5)	Heneicosane	727
30	[illegible]		[illegible]	[illegible]		

TABLE A-69. (Continued)

GC Peak No.	Retention Index	Amount, μg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	SI $\times 10^3$
31	1757	***	C ≥ 17 Alkane	56(100)41(51)69(51)83(29)97(18)111(20)126(7)139(3)156(2)	6-Tridecene, 7-Methyl	757
32	1764	**	C ≥ 17 Alkene	56(100)41(67)70(36)69(34)83(15)97(10)111(6)	1-Octene, 3,7-Dimethyl-	749
33	1780	***	C ≥ 17 Alkene	70(100)55(66)41(56)83(28)97(19)111(9)125(4)	1-Dodecene, 2-Ethyl	575
34	1802	**	Octadecene	55(100)57(85)41(82)43(78)60(70)83(71)97(55)111(23)	1-Octadecene	775
35	1816	**	C ≥ 18 Alkene	57(100)43(80)55(62)71(62)41(60)85(35)97(22)111(11)		
36	1876	**	C ≥ 18 Alkane	57(100)55(95)41(85)43(84)71(60)83(38)97(36)180(2)		
37	1955	**	Heptadecanol	55(100)41(86)43(86)69(72)82(63)97(42)111(20)125(8)196(0.3)	1-Heptadecanol	820
38	1966	**	C ≥ 19 Alkane	57(100)43(87)41(52)71(69)85(61)99(10)113(6)127(4)		
39	1987	**	C ≥ 19 Alkene			
40	1993	**	Eicosene	56(100)55(67)57(66)41(55)69(56)83(36)97(23)111(18)126(9)		
41	2003	**	C ≥ 20 Alkene	56(100)57(57)55(56)41(50)70(41)83(17)97(11)111(8)		
42	2155	**	C ≥ 20 Alkene	55(100)57(89)43(83)41(79)69(71)83(75)97(62)111(27)125(12)	1-Hexadecene	776
43	2196	**	C ≥ 21 Alkene	57(100)43(88)55(72)41(63)71(62)85(35)97(28)111(13)		
44	2292	**	C ≥ 22 Alkane	55(100)57(76)43(84)69(73)83(64)97(46)111(21)		
45	2357	**	C ≥ 23 Alkene	56(100)57(74)55(72)69(58)83(37)97(28)111(19)		
46	2398	**	C ≥ 23 Alkene	55(100)41(79)43(90)57(88)		
47	2553	**	Docosanol	55(100)43(89)41(78)69(72)83(89)97(50)111(22)125(10)	1-Docosanol	673
48	2750	**	C ≥ 27 Alkene	56(100)57(78)55(73)69(59)83(37)97(30)111(20)126(7)139(7)		
49	2969	**	C ≥ 29 Alkene	56(100)57(85)55(79)69(65)83(60)97(39)111(25)195(1.5)		

TABLE A-70. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 29E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10^3
1	910	***	$C \geq 6$ Fatty acid	74(100)43(83)59(47)87(46)99(22)101(11)	Pentenoic acid,3-methyl, methyl ester	548
2	1052	**	$C \geq 7$ Fatty acid	74(100)43(41)41(40)59(23)101(21)127(5)	Hexanoic acid,5-methyl, methyl ester	567
3	1068	**	Benzoic acid	105(100)77(90)51(76)136(27)	Benzoic acid, methyl ester	575
4	1095	**	Methylphenol	107(100)108(90)77(58)79(50)51(34)63(17)	Phenol,2-Methyl	535
5	1164	**	Benzeneacetic acid	91(100)65(24)150(19)63(11)	Benzene acetic acid, methyl ester	584
6	1232	**	Methoxy C_3-Alkylbenzene	135(100)91(69)121(42)150(32)51(24)65(20) [illegible]	Benzene,2-Methoxy-1,3,5-Trimethyl	513
7	1250	**	$C \geq 10$ Fatty acid	74(100)41(44)43(38)101(33)59(24)155(3)	Hexanoic acid,5-methyl, methyl ester	572
8	1364	**	Diphenyl ether	51(100)77(63)141(66)170(65)65(32)115(32)142(44)171(8)	Benzene,1,1'-Oxybis	565
9	1442	**	$C \geq 11$ Fatty acid	103(100)43(98)71(57)79(46)55(31)61(26)127(3)	Tetradecanoic acid,3-Hydroxy, methyl ester	409
10	1496	**	$C \geq 11$ Fatty acid	74(100)87(57)41(48)55(36)115(19)170(20)141(14)183(2)	Nonanoic acid, methyl ester	490
11	1885	**	$C \geq 16$ Fatty acid	55(100)41(95)69(52)74(50)87(31)152(7)194(4)	11-Octadecenoic acid, methyl ester	500
12	1911	**	Hexanoic acid	74(100)87(63)43(53)55(38)143(12)	Heneicosanoic acid, methyl ester	697
13	2080	**	Octadecenoic acid	41(100)55(98)69(50)74(47)87(28)180(2)	10-Undecenoic acid, methyl ester	636
14	2086	**	Octadecenoic acid	55(100)69(53)74(44)87(26)98(16)264(1)	10-Undecenoic acid, methyl ester	590
15	2111	**	$C \geq 18$ Fatty acid	74(100)43(64)87(62)55(42)143(10)199(2)185(1)	Heneicosanoic acid, methyl ester	823

TABLE A-71. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 29E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10^3
1	1123	**	Dimethylaniline	106(100)121(40)77(13)79(8)	Pyridine, 3-Ethyl-5-Methyl	496
2	1198	*	Quinoline	129(100)102(22)128(20)130(10)75(10)63(6)	Quinoline	757
3	1215	*	N-Ethyl-O-Toluidine or C_3-Alkylaniline	120(100)135(36)121(11)91(10)77(9)106(6)		
4	1293	**	Diethylaniline	136(100)149(38)119(20)91(10)77(7)65(3)		

TABLE A-72. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 30VE

GC Peak No.	Relative Retention Time	Amount µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.10	----	Air	44(100)
2	0.10	1-10	Butene	41(100)56(70)
3	0.10	1-10	Acetone +	43(100)58(50)101(30)103(18)101(2)
		1-10	Trichlorofluoromethane	
4	0.11	1-10	Dichloroethylene	61(100)96(67)98(50)
5	0.12	1-10	Dichloromethane	49(100)
6	0.21	1-10	Methyl cyclopentone	56(100)41(62)69(40)84(4)
7	0.22	1-10	1,1,1-Trichloroethane	97(100)61(66)99(65)63(22)117,119(12)
8	0.33	1-10	Trichloroethylene	95(100)130(80)132(70)
9	0.70	1-10	Tetrachloroethene	129(100)131(95)166(95)
10	0.98	1-10	C_2 Alkyl benzene	91(100)106(50)
11	1.00	(8)-	I.S.	75(100)
12	1.18	1-10	C_3 Alkyl benzene	105(100)120(30)
13	1.19	1-10	C_3 Alkyl benzene	105(100)120(30)
14	1.21	1-10	C_3 Alkyl benzene	105(100)120(21)
15	1.31	1-10	C_2 Alkyl benzene	105(100)120(25)
16	1.32	1-10	Methyl styrene	117(100)118(50)115(36)91(20)
17	1.37	1-10	C_4 Alkyl benzene (diethyl) $C_{10}H_{14}$	105(100)119(85)91(30)134(25)
18	1.38	1-10	C_4 Alkyl benzene	105(100)57(40)119(25)134(15)
19	1.39	1-10	C_4 Alkyl benzene (ethyldimethyl)	119(100)91(30)134(20)
20	1.40	1-10	C_4 Alkyl benzene (methyl propyl)	105(100)134(12)
21	1.44	1-10	C_4 Alkyl benzene (ethyl dimethyl)	105(100)91(28)134(20)
22	1.47	1-10	C_4 Alkyl benzene (ethyl dimethyl)	119(100)91(30)105(22)134(15)
23	1.50	1-10	C_4 Alkyl benzene (tetramethyl)	119(100)91(25)134(20)
24	1.51	1-10	C_4 Alkyl benzene	119(100)91(22)134(20)
25	1.55	1-10	Ethyl styrene $C_{10}H_{12}$	117(100)115(30)

TABLE A-73. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 30E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	RI x 10³
1	863	**	Toluene	91(100)92(58)65(16)51(10)	Benzene, Methyl-	563
2	869	***	Ethylbenzene	91(100)106(23)51(16)65(14)77(12)	Benzene, Ethyl	762
3	883	***	O-Xylene	91(100)106(36)77(16)91(15)65(10)	Benzene, 1,2-Dimethyl	698
4	897	***	P-Xylene	91(100)106(34)77(16)51(17)65(11)63(10)	Benzene, 1,4-Dimethyl	533
5	908	**	2-Butoxyethanol	57(100)45(53)41(52)87(18)	Ethanol, 2-Butoxy	884
6	936	**	C3-Alkylbenzene	91(100)65(18)120(15)51(15)	Benzene, Propyl	663
7	942	**	C3-Alkylbenzene	105(100)120(27)77(20)91(17)79(16)51(13)	Benzene, 1-Ethyl-2-Methyl	701
8	948	**	C3-Alkylbenzene	105(100)120(37)91(18)77(23)51(16)63(10)65(10)	Benzene, 1,3,5-Trimethyl	675
9	957	**	C3-Alkylbenzene	105(100)120(38)77(26)79(19)51(16)65(12)63(11)	Benzene, 1-Ethyl-2-Methyl	660
10	976	***	C3-Alkylbenzene	105(100)120(34)77(18)91(16)51(16)79(13)65(9)63(8)	Benzene, 1,2,4-Trimethyl	659
11	1002	**	C3-Alkylbenzene	105(100)120(33)77(19)91(15)51(16)79(14)65(9)63(9)	Benzene, 1,2,4-Trimethyl	654
12	1011	**	Methylstyrene	117(100)118(57)91(32)63(26)51(22)	Benzene, 1-Ethenyl-4-Methyl	668
13	1017	**	C3-Alkenylbenzene	115(100)116(90)63(32)89(22)117(16)	Benzene, 1,2-Propadienyl	615
14	1029	**	?	57(100)59(26)115(14)	Propane, 1-(1,1-Dimethyl Ethoxy)-2-Methyl	603
15	1039	**	C4-Alkylbenzene	119(100)134(29)91(60)105(21)77(22)51(16)65(12)63(10)	Benzene, 2-Ethyl-1,4-Dimethyl	523
16	1057	**	C4-Alkylbenzene	119(100)91(33)134(25)77(20)51(15)65(11)63(10)	Benzene, 2-Ethyl-1,4-Dimethyl	552
17	1064	**	C4-Alkylbenzene	119(100)9(33)134(27)107(22)77(17)51(13)65(12)63(10)	Benzene, 1-Methyl-2-(1-Methyl Ethyl)	611
18	1082	**	C4-Alkylbenzene	119(100)134(38)91(30)77(17)91(12)65(11)63(9)	Benzene, 1,2,4,5-Tetramethyl	522
19	1099	**	C4-Alkylbenzene	119(100)134(36)91(31)77(17)91(16)65(11)63(8)	Benzene, (1-Ethyl, Propyl)	337
20	1122	**	Ethylstyrene	117(100)91(44)132(29)51(26)63(18)65(17)	Benzene, 1-Ethenyl-4-Ethyl	616
21	1128	**	Ethylstyrene	117(100)115(40)132(31)91(23)63(18)65(16)77(16)	Benzene, 1-Ethenyl-4-Ethyl	561
22	1133	**	C4-Alkylbenzene	119(100)134(34)91(30)51(18)63(18)65(18)	Benzene, 1,2,4,5-Tetramethyl	464
23	1151	**	Naphthalene	128(100)102(16)51(18)63(14)129(10)	Naphthalene	618
24	1164	**	C5-Alkylbenzene	133(100)148(24)77(20)119(17)105(18)51(15)91(15)65(10)	Benzene, 1-Ethyl-3-(1-Methylethyl)	715
25	1261	**	Methylnaphthalene	142(100)141(89)115(60)63(20)51(17)	Naphthalene, 2-Methyl	385
26	1276	**	Methylnaphthalene	142(100)141(96)115(65)63(22)51(13)	Naphthalene, 2-Methyl	613
27	1457	**	?	57(100)71(25)167(31)165(27)137(13)	1,6-Octadecadiynoic Acid, Methyl Ester	325

TABLE A-74. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 30E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	SI x 10^3
1	997	*	Dimethyl Aniline	106(100)121(60)120(20)77(26)79(18)	Pyridine, 3-Ethyl-4-Methyl	629
2	1063	**	?	100(100)42(16)56(15)70(16)101(8)145(5)	Urea, Triethyl Nitroso-	348

TABLE A-75. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 31VI

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.12	--	Air	44(100)
2	.16	1-10	Acetone	43(100)58(30)
3	.16	1	Diethyl ether	59(100)45(96)75(55)
4	.17	1-10	Dichloromethane	49(100)84(52)86(35)
5	.17	10-20	Chloropropene	41(100)39(68)76(35)55,78(12)
6	.23	<1	Chloroform	83(100)85(67)
7	.23	<1	Diisopropyl ether or Dipropoxy ethane	45(100)41(43)87(18)59(10)69(5)
8	.25	<1	Tetrahydrofuran + ?	42(100)41(89)55(57)39(43)72(39)71(37)90(10)
9	.26	<1	1,1,1-trichloroethane	97(100)99(67)61(43)119(17)
10	.29	<1	Benzene	78(100)
11	.35	<1	Dichloropropane	63(100)62(75)41(68)39(50)65(30)77(27)76(26)
12	.36	<1	Trichloroethylene	95(100)130(90)132(87)97(62)
13	.68	<1	1,1,2,2-Tetrachloroethene	131(100)166(82)129(78)164(67)
14	1.00	~(8)	I.S.	75(100)77(33)

TABLE A-76. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 31VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.14	--	Air	44(100)
2	0.15	1-10	Butene	41(100)56(40)
3	0.17	10-100	Acetone	43(100)58(25)
4	0.23	10-100	Methylethyl ketone	43(100)72(20)
5	0.29	1-10	1,1,1-Trichloroethane	97(100)99(70)61(45)117,119,121
6	0.31	1-10	Methylisopropyl ketone	43(100)86(12)41(11)71(3)
7	0.31	1-10	Benzene	78(100)
8	0.33	1-10	C_7H_{14}, e.g., 2,3-Dimethyl-1-pentene	41(100)69(95)55(45)70(35)83(20)98(10)
9	0.45	1-10	Unknown hydrocarbon	81(100)41(82)67(65)53(60)79(50)96(68)
10	0.50	1-10	Methylisobutyl ketone	43(100)58(30)57,41(20)85(12)100(5)
11	0.57	1-10	C_7H_{12}, e.g., Methyl hexadiene	81(100)79(50)96(68)53(67)41(60)
12	0.59	1-10	C_7H_{12}	81(100)79(52)96(45)53,41(40)
13	0.62	1-10	C_8H_{16}, e.g., Dimethyl hexene	69(100)41(88)55(40)70(35)112(30)
14	0.66	1-10	Unknown	57(100)41(32)114(11)85(5)71(3)
15	0.70	1-10	1,1,2,2-Tetrachloroethane + unknown	43(100)57(38)85(30)41(28)72(22)129(3)131(2)166(2)
16	0.72	10-100	C_7 Ketone, e.g., 2,4-Dimethyl-3-pentane	43(100)71(30)41(12)55(10)70(9)86(8)
17	0.76	1-10	3-Methyl-2,4-pentanedione (T)	43(100)72(28)71(15)99(3)114(3)
18	0.82	1-10	4,4-Dimethylheptane (T)	43(100)85(30)41(25)71(20)
19	0.83	1-10	Ethyl butylaldehyde (T)	43(100)72(15) M100 $C_6H_{12}O$
20	0.86	10-100	C_8 Ketone, e.g., 4-Methyl-2-heptanone (T)	43(100)58(93)59(30)57(28)41(22)85(15)
21	0.88	10-100	C_2-Alkyl benzene	91(100)106(35)
22	0.96	>100	Cyclooctatetraene (T)	104(100)78(50)103(40)51(33)77(30) Big One
23	0.97	1-10	Trimethyl cyclohexane (T)	109(100)67(68)91(50)124(20)
24	1.04	>100	Unknown	69(100)43(85)41(70)84(50)57(30)
25	1.07	10-100	C_3-Alkyl benzene	105(100)120(25)
26	1.19	1-10	Unknown	67(100)109(95)124(40)
27	1.23	1-10	Unknown	43(100)71(95)70(28)41(38)
28	1.29	>>100	2-Ethyl-1-hexanol	57(100)43(51)41(38)55(35)69(23)83(12)97(2)

TABLE A-77. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 31E

GC Peak No	Retention Index	Amount, μg[a]	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	BI x 10^3
1	807	***	Heptane	43(100)57(60)71(56)70(15)100(10)	Heptane	688
2	818	***	Methylcyclohexane	83(100)55(97)98(39)40(39)56(44)	Cyclohexane, Methyl-	593
3	825	**	C ≥ 8 Alkane	41(100)57(76)69(70)85(28)58(8)1.4(1)	Hexane, 3,4-Dimethyl	369
4	850	**	Toluene	91(100)92(80)65(22)63(15)51(13)50(9)	Benzene, Methyl	542
5	855	**	C ≥ 8 Alkane	43(100)85(66)57(49)71(22)99(6)114(2)		
6	864	**	Alkyl Ether ?	43(100)59(53)85(23)99(15)100(0.6)		
7	869	**	Ethylbenzene	91(100)106(25)107(2)	Benzene, Ethyl	749
8	883	***	Styrene	104(100)78(68)103(48)51(36)105(8)	Benzene, Ethenyl	622
9	924	***	C ≥ 9 Alkane	43(100)41(98)69(94)84(68)101(2)104(1)	Hexane, 2,3,3,3-Tetra-Methyl	619
10	935	***	C_3-Alkylbenzene	105(100)120(21)77(27)79(23)51(22)43(17)	Benzene, (1-Methyl Ethyl)-	661
11	982	***	C_3-Alkylbenzene + ?	57(100)77(94)41(88)105(69)106(65)120(1)125(1)		
12	1031	***	Methylheptanol	57(100)43(96)55(88)41(78)69(82)70(50)83(36)84(32)97(12)	1-Heptanol, 6-Methyl-	898
13	1061	**	Alkyl-Alcohol C ≥ 8	55(100)41(99)56(98)69(60)84(41)122(1)	1-Octanol	772
14	1082	**	Alkyl-Alcohol or Alkene	43(100)55(77)41(72)57(63)69(54)83(24)121(21)	1-Heptanol, 6-Methyl	637
15	1087	**	Alkyl-Alcohol or Alkene	57(100)41(73)69(70)55(50)83(12)111(6)	1-Heptanol, 6-Methyl-	616
16	1108	**	Alkyl-Alcohol or Alkene	69(100)55(98)41(87)83(29)97(14)	4-Decene	670
17	1119	**	Alkyl-Alcohol or Alkene Mixture	43(100)59(55)101(52)57(50)85(26)83(19)127(4)		
18	1137	**	Alkyl-Alcohol or Alkene	43(100)45(49)73(46)55(45)87(38)131(0.8)	3-Hexanol, 2,4-Dimethyl	577
19	1164	**	Alkyl-alcohol or Alkene	55(100)41(70)69(56)57(42)97(30)83(24)115(3)	1-Heptanol, 6-Methyl-	746
20	1187	**	C ≥ 12 Alkene	41(100)55(94)69(95)83(68)57(65)	1-Pentadecene, 2-Methyl-	736
21	1193	**	Alkyl-Alcohol or Alkene	57(100)41(81)69(83)56(59)55(57)112(12)	1-Decanol	787
22	1201	**	Alkyl-Alcohol or Alkene	55(100)41(80)69(76)83(25)112(17)111(15)	Isooctane, (Ethenyloxy)-	560
23	1207	**	Alkyl-Alcohol or Alkene	69(100)43(79)41(77)70(55)55(53)112(16)	1-Heptene, 6-Methyl	623
24	1217	**	Alkyl-Alcohol or Alkene	55(100)41(44)83(39)69(21)97(18)	1-Nonene	527
25	1229	**	1-Phenyl-1-Propanol	77(100)105(99)51(51)136(2)		
26	1361	**	Subst.-Styrene	104(100)78(28)51(13)178(2)165(1)		
27	1690	*	?	91(100)57(73)43(68)41(52)71(46)130(17)208(6)		
28	1718	**	Subst.-Styrene	104(100)78(22)51(10)178(4)179(1)		
29	2408	**	Subst.-Benzene	91(100)117(20)65(14)77(12)51(6)207(5)208(2)		
30	2498	**	Subst.-Benzene	91(100)179(66)207(26)105(23)77(20)206(17)208(6)		

TABLE A-77. (Continued)

GC Peak No	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10^3
31	2516	+++	Subst.-Benzene	91(100)129(63)207(23)77(19)206(10)208(4)		
32	2529	++	Subst.-Benzene	91(100)129(70)207(30)105(25)77(22)		
33	2611	++	Subst.-Benzene	91(100)129(40)106(37)77(20)65(16)207(9)208(9)		

TABLE A-78. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 31E

GC Peak No.	Retention Index	Amount, μg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	R.I. x 10^3
1	838	**	C ≥ 6 Fatty acid	74(100)43(31)59(28)99(15)101(14)	Pentanoic acid,3-methyl-methyl ester	541
2	842	*	C ≥ 6 Fatty acid	74(100)87(63)55(51)43(48)57(42)99(30)104(22)	Pentanoic acid,4-Methyl-methyl ester	477
3	852	**	C ≥ 6 Fatty acid	88(100)43(36)87(38)101(36)69(25)74(19)113(8)		
4	868	**	C ≥ 7 Fatty acid	88(100)57(33)41(27)87(19)69(17)113(6)115(5)	Heptanoic acid,2,6-Dimethyl, methyl ester	475
	868	**	C ≥ 7 Fatty acid	88(100)57(26)41(18)59(16)87(11)115(6)113(5)		
5	878	**	C ≥ 7 Fatty acid	74(100)87(74)43(41)59(35)69(33)101(32)113(20)129(2)	Heptanoic acid, methyl ester	419
6	882	**	C ≥ 7 Fatty acid	74(100)43(36)59(27)73(26)101(24)113(14)	Hexanoic acid,5-methyl, methyl ester	434
7	893	**	C ≥ 7 Fatty acid	87(100)74(99)55(67)41(46)73(41)59(36)115(28)113(24)		
8	900	**	C ≥ 7 Fatty acid	87(100)102(61)55(30)57(22)115(19)130(10)143(2)		
9	902	**	C ≥ 7 Fatty acid	87(100)107(64)116(44)57(35)127(4)129(4)	Heptanoic acid,2-Propyl,methyl ester	445
10	912	**	C ≥ 7 Fatty acid	88(100)101(32)57(28)69(24)41(23)129(8)127(5)		
11	928	***	C ≥ 7 Fatty acid	74(100)101(34)43(26)59(20)88(19)127(6)143(2)		
12	940	**	C ≥ 7 Fatty acid + ?	69(100)41(54)87(56)55(43)84(36)116(18)		
13	942	**	C ≥ 7 Fatty acid + ?	88(100)57(62)41(37)74(42)111(26)127(15)143(12)		
14	948	**	C ≥ 8 Fatty acid	87(100)102(70)41(38)55(36)57(34)69(28)130(12)		
15	957	***	C ≥ 8 Fatty acid	74(100)87(37)55(34)43(28)609(23)115(15)127(11)		
16	974	***	C ≥ 8 Fatty acid	74(100)87(65)41(38)69(34)101(32)55(27)59(25)127(14)129(8)		
17	981	***	C ≥ 8 Fatty acid	74(100)101(32)59(16)69(14)87(11)127(10)143(1)		
18	996	***	C ≥ 8 Fatty acid	74(100)55(74)115(75)83(68)87(64)59(34)109(26)127(12)		
19	1005	****	Benzoic acid	105(100)77(66)136(36)51(21)115(4)	Benzoic acid, M.E.	572
20	1061	**	C ≥ 8 Fatty acid	74(100)101(60)41(30)55(28)115(14)123(10)141(6)	Nonanoic acid, methyl ester	438
21	1069	**	C ≥ 8 Fatty acid	87(100)74(58)55(48)57(44)99(18)115(14)141(9)157(2)		
22	1089	**	C ≥ 9 Fatty acid	88(100)101(99)87(82)41(48)69(48)43(41)129(20)141(7)143(6)	Undecanoic acid,2-methyl, methyl ester	506
23	1097	**	C ≥ 9 Fatty acid + ?	87(100)101(88)74(74)55(65)102(73)111(46)143(46)		
24	1105	**	C ≥ 9 Fatty acid	88(100)101(68)69(37)43(37)55(36)129(19)143(10)	Heptanoic acid,2-ethyl	456
25	1119	**	C ≥ 9 Fatty acid	74(100)55(62)67(61)41(53)97(40)115(38)129(34)143(4)		
26	1135	**	C ≥ 9 Fatty acid + ?	74(100)88(29)55(27)87(20)129(17)143(17)155(3)157(3)	Decanoic acid, methyl ester	450
27	1159	**	C ≥ 9 Fatty acid	74(100)55(46)83(40)88(37)115(30)87(25)157(18)		
28	1163	**	C ≥ 9 Fatty acid	74(100)101(48)55(24)69(24)137(8)155(4)157(3)		
29	1166	**	C ≥ 9 Fatty acid	74(100)115(38)55(26)43(22)157(20)143(8)		

TABLE A-78. (Continued)

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	RI x 10^3
30	1169	**	C ≥ 9 Fatty acid	74(100)101(49)69(26)55(19)59(18)143(8)	Hexanoic acid,5-methyl-methyl ester	410
31	1174	**	C ≥ 9 Fatty acid	74(100)87(95)55(55)69(47)113(30)143(18)155(8)157(6)	Tetradecanoic acid,12-methyl-methyl ester	415
32	1176	**	C ≥ 9 Fatty acid	74(100)101(83)55(30)69(29)87(30)143(7)155(6)171(2)		
33	1186	**	C ≥ 9 Fatty acid + ?	74(100)101(86)55(33)97(22)87(20)143(5)155(4)157(3)		
34	1190	***	C ≥ 9 Fatty acid	87(100)74(67)55(52)97(26)143(8)155(4)157(2)		
35	1199	***	C ≥ 9 Fatty acid	87(100)74(54)55(46)57(38)97(23)155(4)		
36	1203	**	C ≥ 10 Fatty acid	87(100)74(54)55(46)113(15)143(5)155(6)171(1)		
37	1211	**	C ≥ 10 Fatty acid	101(100)87(99)75(81)102(67)69(62)113(37)155(36)143(6)		
38	1215	**	C ≥ 10 Fatty acid	74(100)87(60)97(60)69(57)55(56)41(47)129(42)137(17)		
39	1217	**	C ≥ 10 Fatty acid	74(100)55(80)83(65)87(39)111(35)143(28)		
40	1221	**	C ≥ 10 Fatty acid	74(100)115(56)55(48)87(40)83(36)137(14)143(3)		
41	1232	**	C ≥ 10 Fatty acid	129(100)97(66)69(65)87(56)74(47)41(41)55(40)137(11)	Octanedioic acid, dimethyl ester	420
42	1236	**	C ≥ 10 Fatty acid	129(100)97(66)69(60)74(56)87(55)55(43)137(11)		
43	1238	**	C ≥ 10 Fatty acid	111(100)83(99)74(82)55(81)87(67)143(56)154(4)		
44	1911	**	Hexanoic acid	74(100)87(85)55(28)143(24)227(6)	Dodecanoic acid,10-Methyl-Methyl ester	396
45	1978	**	?	134(100)107(32)79(29)57(26)166(21)167(21)234(5)		
46	2080	**	C ≥ 18 Fatty acid	55(100)69(72)74(70)83(62)87(54)97(56)180(10)266(8)	10-Octadecenoic acid, methyl ester	441
47	2111	**	C ≥ 18 Fatty acid	74(100)87(86)143(31)55(29)199(16)	Heneicosanoic acid, methyl ester	537
48	2230	**	Subst. phenanthrene carboxylic acid	171(100)91(24)105(19)241(3)316(2)		
49	2512	**	Subst. phenanthrene carboxylic acid	121(100)81(35)107(30)189(27)302(3)303(2)347(1)		

TABLE A-79. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 31E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	RI x 10^3
			Neutral compounds were so concentrated that they were also extracted into basic fraction.			
			No basic compounds were identified in this fraction.			

TABLE A-80. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 32VE

GC Peak No	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.19	----	Air	44(100)
2	0.24	10-100	Dichloromethane	49(100)
3	0.25	10-100	Cyclopentadiene	66(100)65(70)40(40)
4	0.25	1-10	Cyclopentene	67(100)68(65)53(20)
5	0.26	1-10	1 Pentene	42(100)55(35)70(25)
6	0.30	10-100	Cloroform	83(100)85(70)82(40)47(38)53(30)85(10)
7	0.33	1-10	Benzene	78(100)
8	0.35	1-10	C_6H_8 eg Cyclohexadiene	79(100)80(50)77(45)
9	0.35	1-10	C_6H_8 eg Cyclohexadiene	79(100)80(55)
10	0.36	1-10	C_6H_{10} eg 2,4-Hexadiene	67(100)82(22)41(21)
11	0.40	1-10	Cyclohexene	67(100)54(70)82(35)41(33)
12	0.43	1-10	Bromodichloromethane	83(100)85(70)47(28)127,129,131
13	0.44	1-10	Tetramethyl butane (T)	57(100)41(32)56(30)43(22)
14	0.59	1-10	Unknown	43(100)71(48)70(30)84(29)91(18)96(13) (Weak spectrum)
15	0.83	1-10	C_8H_{12} eg 4-Vinylcyclohexene	54(100)79(60)66(40)80(30)
16	1.34	1-10	Dicyclopentadiene	66(100)65(20)

TABLE A-81. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 32E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	KI x 10³
1	862	**	C_3-Alkylbenzene	105(100)91(66)51(38)120(36)77(35)		
2	867	**	C_3-Alkylbenzene	105(100)91(76)51(37)120(35)77(38)	Benzene,1-Ethyl-2-Methyl	431
3	881	**	?	66(100)51(11)78(7)77(6)		
4	948	**	Indene	115(100)116(90)89(22)63(35)51(20)	1H-Indene	398
5	957	**	Methylindene	115(100)130(73)51(35)63(29)77(26)117(29)131(13)	1H-Indene,3-Methyl	368
6	972	**	Methylindene ($C_{10}H_{10}$) + C_4-Alkylbenzene	115(100)130(82)129(62)51(28)63(26)77(20)		
7	1151	**	Naphthalene + ?	128(100)102(15)51(16)63(16)76(12)129(12)	Azulene	558
8	1191	***	Tetrahydrothiophene 1,1-Dioxide ($C_4H_8O_2S$) + Sulfur containing compound	41(100)56(56)55(50)120(34)64(8)	Thiophene,tetrahydro-1,1-dioxide	416
9	1263	**	Methylnaphthalene	142(100)141(89)115(61)63(20)89(12)51(12)143(13)	Naphthalene,2-methyl	369
10	1276	**	Methylnaphthalene	142(100)141(96)115(64)63(21)89(12)74(11)143(12)	Naphthalene,2-methyl	437
11	1288	**	Dihydro dimethylindene	131(100)146(58)115(42)103(37)63(35)51(25)77(23)91(20)	1H-Indene,2,3-dihydro-4,6-dimethyl	362
12	1306	**	Tetrahydrodimethylnaphthalene	115(100)117(97)160(52)43(41)145(37)91(35)63(31)	Naphthalene,1,2,3,4-tetrahydro-1-1-dimethyl	340
13	1398	**	Alkyl alcohol C ≥ 12	69(100)84(87)43(62)55(46)131(8)174(5)		
14	1433	**	Subst. alkylbenzene + ?	104(100)77(36)91(25)63(19)51(18)69(15)148(12)		
15	1481	**	Subst. alkylbenzene ?	117(100)118(92)91(32)77(26)51(21)63(18)162(6)		
16	1553	**	Mixture ?	98(100)79(71)77(47)70(31)41(29)152(26)175(31)		
17	1633	**	Subst. alkylbenzene + ?	91(100)77(92)51(60)105(55)130(55)144(40)172(25)190(12)		
18	1700	**	Subst. alkylbenzene	91(100)77(78)79(71)117(60)143(55)65(40)186(22)204(22)		

TABLE A-82. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 32E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10^3
1	1078	**	?	66(100)91(22)65(19)55(16)77(14)121(5)152(4)		
2	1085	**	?	66(100)91(22)65(20)55(18)77(12)121(5)152(5)		
3	1166	***	?	41(100)56(62)55(54)120(18)48(24)64(23)		
4	1280	*	Hydroxybenzoic acid	134(100)106(48)105(67)77(66)166(44)135(30)	Benzoic acid,2-hydroxy-6-methyl,methyl ester	564
5	1321	**	?	172(100)157(72)97(63)113(58)125(48)79(41)59(34)45(27)		
6	1338	**	?	95(100)126(90)91(36)77(24)168(14)167(8)		
7	1343	**	Subst. naphthalene	186(100)59(66)171(60)127(53)139(42)45(21)		
8	1351	**	Subst. naphthalene	186(100)171(64)111(50)127(46)139(46)59(42)		
9	1356	**	Subst. naphthalene	186(100)111(66)171(46)59(35)93(31)127(30)155(18)		
10	1361	**	?	117(100)188(59)111(64)115(62)59(46)77(22)171(25)		
11	1555	**	?	129(100)128(88)188(39)127(36)153(28)212(4)		
12	1692	**	?	126(100)79(76)77(56)175(59)167(24)202(7)		

TABLE A-83. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 32E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10^3
1	1109	*	C_4-Alkylpyridine	135(100)136(61)120(26)79(18)77(15)91(15)	Pyridine, 4(1,1-Dimethyl Ethyl)-	263
2	1172	***	Mixture, Sulfolene + ?	41(100)56(59)55(54)120(50)64(18)148(10)149(5)	Thiophene, Tetrahydro	394
3	1225	*	Dimethylquinoline	157(100)115(20)142(13)156(23)158(13)89(8)	Quinoline, 2,4-Dimethyl	600
4	1232	*	Mixture ?	131(100)121(78)103(52)91(62)77(28)146(40)206(2)	1H-Indene-1,2-Diol,2,3-Dihydro-1-Methyl	583

TABLE A-84. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 33VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.11	----	Air	44(100)
2	0.14	<1	Butene	41(100)56(66)
3	0.16	1-10	Acetone	43(100)58(25)
4	0.16	1-10	Diethyl ether	59(100)74(72)45(70)
5	0.16	1-10	Dichloroethylene	61(100)96(60)63(30)98(28)
6	0.17	10-100	Dichloromethane	49(100)
7	0.17	1-10	Dicyclopentadiene	66(100)65(70)40(48)
8	0.21	<1	Methyl ethyl ketone	43(100)72(20)
9	0.21	1-10	Diisopropylether	45(100)43(68)87(20)59(10)
10	0.26	<1	1,1,1-Trichloroethane	97(100)99(60)61(60)117,119,121
11	0.28	<1	Benzene	78(100)
12	0.31	1-10	1,2-Dichloropropane	63(100)62(68)41(65)76(60)
13	0.38	<1	Methyl-t-butyl Ketone	57(100)41(70)43(68)100(15)55(10)
14	0.47	<1	C_8H_{16} eg 2,4,4-tri-methyl-1-pentane	57(100)41(55)55(35)69(10)97(10)112(10)
15	0.48	<1	C_8H_{16}	55(100)97(50)41(65)69(25)112(20)
16	0.81	<1	C_8H_{16}	55(100)83(90)41(65)69(30)
17	0.92	<1	C_2 Alkyl benzene	91(100)106(40)
18	1.00	8 -	I S	75(100)
19	1.21	<1	C_3 Alkyl benzene	105(100)120(35)
20	1.23	1-10	C_4 Alkyl benzene	119(100)91(28)134(20)
21	1.44	<1	C_4 Alkyl benzene	119(100)91(30)134(20)

TABLE A-85. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 33E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	RI x 10^3
1	861	**	Toluene	91(100)92(84)65(24)51(16)93(8)	Benzene,Methyl-	560
2	867	**	Alkyl-ether	59(100)57(60)41(22)43(19)115(3)97(1)	Propane,1-(1,1-dimethyl ethoxy)-2-methyl	508
3	870	**	Ethyl benzene	91(100)106(48)105(19)77(19)63(10)		
4	895	**	Alkyl-ether	43(100)41(75)57(96)59(74)55(36)72(59)71(42)101(12)	Methane,tert-butoxyisopropoxy	529
5	906	**	C = 9 Alkene C_9H_{16}	67(100)109(50)41(44)43(42)81(39)126(19)		
6	998	**	Alkenyl alcohol or Alcohol	43(100)72(66)57(51)41(32)83(9)85(4)99(6)	Pentane,1-(1-butenyloxy)-	631
7	1028	**	(Methylnonene) $C_{10}H_{20}$	41(100)55(96)69(56)85(59)109(29)120(8)160(19)		
8	1036	**	C_4-Cyclohexanol $C_{10}H_{20}O$	66(100)109(64)81(56)41(50)43(49)57(40)81(58)126(27)138(6)	Cyclohexanol,4-sec-butyl	356
9	1068	**	C_3-Cyclohexanone $C_9H_{16}O$	67(100)95(88)96(56)41(47)81(45)110(29)138(35)139(3)	2-Cyclohexen-1-one,3,4,4-trimethyl-	653
10	1076	**	C_3-Cyclohexenone	123(100)95(83)67(58)41(34)55(22)110(19)138(35)139(4)	Cyclohexanone,2-(1-methylethylidene)-	405
11	1090	**	C_3-Cyclohexadienone	79(100)77(42)136(4)	2,5-Cyclohexadien-1-one,3,4,4-trimethyl	361
12	1223	**	Alkylcyclohexanone	43(100)41(67)56(75)69(52)86(21)99(15)116(13)126(8)	Cyclohexanone,4-ethyl	536
13	1277	**	Mixture ?	56(100)41(78)85(24)55(25)121(7)169(2)140(0.2)		
14	1288	**	Isomer of #13 ?	56(100)41(76)85(18)121(6)169(5)		
15	1395	**	?	77(100)65(99)91(85)111(58)156(55)		
16	1432	**	Alkyl-indene	41(100)83(84)69(85)84(80)55(78)57(75)165(45)180(20)221(3)		
17	1460	**	?	69(100)43(62)41(50)84(44)55(37)127(8)191(3)205(2)		
18	1479	**	?	69(100)41(58)55(58)84(16)95(18)177(8)		
19	1548	**	Nonanethiol	55(100)56(86)69(88)41(60)86(36)98(16)160(7)	1-Nonanethiol	595
20	1560	**	Alkyl-alcohol	41(100)70(85)55(63)69(57)83(15)163(11)	4-Undecanol,7-ethyl-2-methyl-	469

TABLE A-86. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 33E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	ΣI x 10^3
1	961	**	?	57(100)101(68)41(54)116(28)73(20)157(7)87(6)		
2	997	**	C ≥ 6 Fatty acid	41(100)57(64)101(72)116(70)73(21)97(11)87(4)157(2)		
3	1004	**	?	41(100)115(100)57(40)130(38)43(34)59(31)83(22)102(22)		
4	1017	**	?	66(100)55(24)91(18)87(16)121(6)152(3)		
5	1026	**	Isomer of #4	66(100)55(15)91(10)87(9)77(8)121(4)152(3)		
6	1037	**	?	102(100)43(69)41(61)73(50)85(35)87(30)143(2)157(1)		
7	1044	**	?	80(100)79(60)55(14)91(10)65(5)135(3)		
8	1100	**	Homolog of #6	102(100)43(45)41(34)87(23)71(16)55(14)127(2)163(1)		
9	1119	**	Homolog of #3	71(100)115(59)43(59)57(51)130(36)143(8)158(3)		
10	1126	***	C ≥ 8 Fatty acid + ?	101(100)41(56)55(40)69(32)116(36)130(10)144(6)157(2)	Hexenoic acid,2-Methyl-2-Propyl-methyl ester	424
11	1132	**	C ≥ 8 Fatty acid	101(100)41(96)130(27)71(25)43(25)115(14)144(6)		
12	1138	**	?	116(100)41(99)71(51)55(42)101(96)127(18)157(3)158(2)		
13	1187	**	C ≥ 8 Fatty acid	101(100)116(56)43(56)41(48)115(32)158(8)157(4)		
14	1362	**	?	102(100)57(66)41(42)43(30)71(36)83(26)115(18)171(3)		

TABLE A-87. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 33E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	ΣI x 10^3
1	859	**	Methylpyridine	93(100)96(7)66(30)65(29)63(21)	Pyridine, 4-Methyl-	607
2	964	**	Trimethylpyridine	121(100)120(31)79*22)77(14)106(19)122(10)	Pyridine, 2,3,5-Trimethyl	536
3	980	***	Trimethylpyridine	121(100)120(74)79(26)77(18)51(12)106(18)122(9)	Pyrridine, 2,3,5-Trimethyl	438
4	1100	**	2,6-Dimethyl-4-Ethylpyridine	135(100)134(66)120(30)91(16)79(16)77(14)136(10)	Methanamine, N-(Phenylmethylene) N-Oxide	265
5	1112	**	C_4-Alkylpyridine (Isomer of #4)	135(100)134(62)120(25)79(17)77(14)91(14)136(10)	Pyridine, 4-(1,1-Dimethyl Ethyl)-	253
6	1190	**	? MW 129	43(100)57(64)81(54)114(50)129(64)128(8)		
7	1205	**	C_5-Alkylpyridine MW 149	148(100)149(46)150(4)121(18)91(9)77(10)	7(1H)-Pteridinone	350
8	1259	**	Mixture ? MW 149	41(100)56(95)85(43)121(22)149(16)		
9	1299	**	Alkylthiophene	125(100)140(81)97(80)51(43)77(39)109(17)141(8)	Thiophene, 2-(1,1-Dimethyl Ethyl)	208

TABLE A-88. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 34VE

GC Peak No	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.13		Air	44(100)
2	0.14	10-100	C_4H_8	56(100)41(70)55(45)
3	0.16	1-10	Furan	68(100)69(3)
4	0.17	1-10	Dichloromethane	49(100)
5	0.22	10-100	Chloroprene	53(100)88(98)50,51(48)90(30)
6	0.24	10-100	Dihydrofuran	70(100)41(70)40,42(40)69(32)
7	0.24	10-100	Chloroprene	53(100)88(75)50(30)51(30)90(90)
8	0.25	1-10	Chlorobutane	55(100)90(50)53(38)92(20)
9	0.27	1-10	Croton aldehyde or dihydro pyron	70(100)41(70)69(45)
10	0.27	1-10	C_4H_6O + 1,1,1-trichloroethane	70(100)41(68)97(80)99,101,117,119,121
11	0.29	1-10	Benzene	78(100)
12	0.44	1-10	C_8H_{16}, e.g., 2,4,4-Trimethyl-1-pentene	57(100)41(48)112(28)97(20)
13	0.48	1-10	C_8H_{16}	97(100)112(40)55(38)69,41(15)
14	0.51	10-100	Chlorobutene + Dichlorobutane (M126)	63(100)62(98)55(60)96(40)
15	0.55	10-100	Dichlorobutane + Chlorobutene	63(100)62(98)55(48)90(40)
16	0.58	10-100	Dichlorobutene (M124)	75(100)58(50)89(45)77(30)
17	0.61	10-100	1,2-Dichlorobutane (M126)	55(100)77(82)41(68)71(40)96(22)
18	0.61	1-10	Dichlorobutane	55(100)41,77(80)62,76(35)90(20)
19	0.90	1-10	$C_4H_6Cl_2$, e.g., 1,1-Dichloro-2-methylene propane	88(100)70(50)53(48)90(33) See 124,126,128
20	0.97	10-100	1,4-Dichlorobut-2-ene	75(100)53(70)89(60)88(55)77(33)62(28)124(20),126,128
21	1.00	8-	I.S.	75(100)
22	1.21	1-10	Tri-isobutene	57(100)41(25)97(20)112(15)168(14)
23	1.23	10-100	Unknown	97(100)57(55)112(25)41(22)69(20)83(18)168(12)
24	1.40	1-10	C_8H_9Cl, e.g., (1-Chloroethyl) benzene	105(100)140(50)103(40)77(30)112(25)142(20)
25	1.58	-100	Unknown	113(100)105(60)88(55)77(40)141(20)176(5)
26	1.59	1-10	1,5-Dichloro-cycloocta-1,5-diene (T)	88(100)53(40)105(30)161(25)

TABLE A-89. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 34E

GC Peak No	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	RI x 10^3
1	886	**	Ethylbenzene	59(100)43(96)91(80)106(24)		
2	896	**	O-Xylene	91(100)106(71)59(32)57(30)43(28)77(24)92(16)	Benzene,1,4-Dimethyl	376
3	907	**	P-Xylene	91(100)106(69)43(20)105(21)77(16)57(15)	Benzene,1,2-dimethyl	486
4	997	**	1-Propene,2-methyl trimer	57(100)41(56)97(13)112(7)168(6)		544
5	1007	**	1-Propene,2-methyl trimer	97(100)57(98)41(72)69(40)83(24)112(23)168(10)	1-Propene,2-methyl,trimer	582
6	1187	***	Chloro- ? Mixture	123(100)55(90)70(86)77(54)95(30)105(23)158(7)160(2)		
7	1208	**	Isomer of #6	123(88)77(96)53(95)70(92)95(76)105(62)158(18)160(6)		
8	1212	**	1-Chloro-5-(1-chloroethenyl) cyclohexene	88(100)105(92)51(70)141(59)113(44)143(18)176(16)178(11)	Cyclohexene,1-chloro-5-(1-chloroethenyl)	603
9	1225	**	Isomer of #8	67(100)123(99)102(75)53(68)88(60)176(4)178(1)		
10	1231	**	Isomer of #8	67(100)88(83)123(76)53(66)95(69)102(31)158(12)160(4)		
11	1266	**	?	43(100)112(92)97(63)69(60)67(39)125(15)146(12)	1-Heptyne,3-ethoxy-3,4-dimethyl	481
12	1286	**	Alkyl-ketone C ≥ 10	43(100)127(20)111(16)85(14)71(14)153(2)168(1)		
13	1311	***	1,3-Butadiene,2-chloro, dimer	88(100)53(96)105(60)141(58)91(45)143(18)176(11)178(0.4)	1,3-Butadiene,2-chloro-dimer	422
14	1317	**	1,Propene,2-methyl-tetramer	57(100)41(36)55(16)97(10)83(8)113(8)140(1)	1-Propene,2-methyl,tetramer	546
15	1339	**	Isomer of #13	57(100)41(34)55(32)97(31)70(20)112(16)176(1)178(0.6)		
16	1351	**	?	104(100)106(38)41(18)53(17)157(5)158(1)		
17	1363	**	?	104(100)77(75)157(61)91(58)51(48)159(20)192(3)196(2)		
18	1375	**	?	104(100)106(32)69(26)53(20)157(12)159(4)		
19	1393	**	Acetic acid C ≥ 8 ester	84(100)69(97)41(59)43(46)70(37)55(32)157(0.4)	Acetic acid, octyl ester	510
20	1637	**	Acetic acid C ≥ 9 ester	84(100)69(96)41(95)43(78)55(40)68(6)180(2)177(1)		

TABLE A-90. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 34E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	SI x 10^3
1	842	**	C ≥ 6 Fatty acid	67(100)41(76)59(65)95(36)96(32)126(32)111(9)		
2	1017	**	?	66(100)55(13)91(11)93(5)121(6)152(3)	4-Pentenoic acid,2-methylene,methyl ester	202
3	1026	**	Methyl cyclohexene-1-carboxylic acid	79(100)67(65)61(46)95(37)122(31)154(26)		
4	1042	**	?	80(100)79(63)55(15)91(10)135(3)93(3)	3-Cyclohexene-1-carboxylic acid,4-methyl methyl ester	326
5	1090	**	?	109(100)68(89)67(76)93(49)136(16)168(6)		
6	1115	**	?	70(100)55(50)123(49)77(13)95(9)79(7)158(6)		
7	1211	**	Alkylphenol	96(100)79(78)65(16)121(12)55(10)121(12)152(6)180(3)		
8	1226	**	Subst. Benzenesulfonic acid	91(100)151(100)65(31)59(25)155(11)185(2)		
9	1263	**	Subst. Benzenesulfonic acid	91(100)158(27)65(27)59(16)127(16)171(2)		
10	1276	**	Subst. Benzenesulfonic acid	91(100)151(57)65(27)59(26)77(16)		
11	1316	**	Benzenesulfonic acid-4-methoxy hydrazide	91(100)127(19)125(18)65(18)151(9)188(3)		
12	1324	***	?	95(100)126(78)91(44)77(20)148(10)186(1)188(0.5)		
13	1353	**	?	151(100)91(36)65(18)155(10)186(5)188(2)		
14	1362	**	?	91(100)65(18)118(22)151(14)186(18)188(4)		
15	1374	**	?	91(100)65(24)77(20)154(40)125(29)127(18)186(28)188(10)		
16	1380	**	?	151(100)91(67)65(20)51(14)155(16)186(8)188(3)		
17	1502	**	?	145(100)129(91)117(82)115(81)91(86)77(43)		
18	1696	***	?	126(100)79(98)175(47)		
19	1726	**	?	79(100)97(53)77(35)91(30)126(20)67(13)175(41)		
20	1815	**	C ≥ 15 Fatty acid	74(100)87(76)		
21	2385	**	?	137(100)79(63)77(46)91(44)216(18)191(15)217(8)	Pentadecanoic acid,14-methyl,methyl ester	324
22	2425	**	?	79(100)137(86)77(61)91(60)43(38)216(18)276(6)		

TABLE A-91. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 34E

GC Peak No	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10^3
1	911	**	?	55(100)121(67)79(66)94(58)42(41)107(16)122(6)		
2	1162	***	Mixture ?	123(100)70(84)55(52)77(26)105(20)158(6)		
3	1541	*	1,3,5-Triazine-2,4-Diamine,	88(100)116(61)60(50)201(60)168(28)	1,3,5-Triazine-2,4-Diamine, 6-(3- Methyl	300
			6-(3-Methyl Phenyl) + ?		Phenyl)-	
4	1642	*	C_5-Alkylquinoline	170(100)199(92)198(36)144(27)77(22)51(18)200(12)		
5	2002	*	Phenothiazine	199(100)167(32)154(13)198(20)200(14)	10H-Phenothiazine	580

TABLE A-92. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 35VI

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.14	--	Air	44(100)
2	.18	1-10	Dichloromethane	84(100)
3	.23	10-100	Chloroform	83(100)85(67)
4	.28	.1-1	Benzene	78(100)
5	.34	1-10	Bromodichloromethane	83(100)85(63)129(8)127(6)
6	1.00	8	I.S.	75(100)110(30)

TABLE A-93. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 35VE

GC Peak No.	Relative Retention Time	Amount, μg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.13	----	Air	44(100)
2	0.20	1-10	Dichloromethane +	49(100)
		1-10	Diethyl ether	59(100)45(45)74(35)
3	0.26	10-100	Chloroform	83(100)85(96)
4	0.30	10-100	Dichloroethane	62(100)64(35)98,100
5	0.39	1-10	1,2-Dichloropropane	63(100)62(70)76(60)41(38)65(32)97,99,101,112,114,116
6	0.57	1-10	Toluene	91(100)92(60)
7	0.72	1-10	1,1-di-sec-Butoxy ethane	45(100)57(60)59(30)101(30)41(28)83(8)
8	0.74	1-10	$C_{10}H_{22}O_2$ (T)	45(100)57(70)101(32)41(30)59(25)83(8)
9	0.80	<1	Hydrocarbon M126	55(100)69(70)56(65)41(60)43(28)70(22)126(9)
10	0.91	~1	C_2 Alkyl benzene	91(100)106(60)
11	0.98	1-10	C_2 Alkyl benzene	91(100)106(55)
12	1.00	~ 8	I S	75(100)77(33)
13	1.19	1-10	Butyl ketone $C_9H_{18}O$	85(100)57(75)142,41(30)58(18)127(15)
14	1.21	~1	Unknown	43(100)86(70)69(40)85(35)99(12)
15	1.22	1-10	C_9H_{10} eg Methyl styrene	117(100)118(80)115(45)91(25)103(10)
16	1.26	1-10	C_9H_{10} eg Methyl styrene	117(100)118(90)115(40)91(22)103(5)
17	1.29	<1	C_3 Alkyl benzene	105(100)120(52)
18	1.32	1-10	C_9H_8 eg Indene	115(100)116(95)117(10)89(10)
19	1.52	<1	$C_{10}H_{10}$ eg cycloprop(2,3)indene or divinyl benzene	130(100)129(85)128(50)115(88)102(8)
20	1.53	1-10	$C_{10}H_{10}$ eg Divinyl benzene	130(100)115(95)129(85)128(40)
21	1.63	~1	Unknown	95(100)137(100)123(80)43(55)109(30)81(27)91(25)41,107,121(14)
22	1.76	1-10	Unknown	125(100)83(70)111(45)55(38)69(30)41(23)126(20)97(10)167(8)
23	1.82	<1	Unknown	141(100)88(87)105(50)143(35)90(30)53(28)113(15)

TABLE A-94. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 35E

GC Peak No	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	RI x 10^3
1	845	**	Toluene	92(100)91(95)	Benzene,methyl	493
2	848	**	Dimethylpentanone	57(100)43(95)58*82)114(17)99(10)86(6)71(6)	2-Pentanone	603
3	868	**	Methylcyclohexenone	83(100)55(87)98(37)	3-Hexen-2-one	571
4	886	**	C_3-Ketone	57(100)59(99)85(32)101(14)116(12)	2,4-Pentanedione	339
5	890	**	Dimethylpentanol	73(100)87(68)55(45)45(39)69(26)101(8)	3-Pentanol	879
6	914	**	O-Xylene	91(100)106(39)77(14)51(13)65(10)63(8)	Benzene,1,2-dimethyl	696
7	921	**	Xylene	91(100)106(39)67(15)51(13)53(11)	Benzene,1,2-dimethyl	463
8	931	**	Dichloropropene	75(100)77(32)110(30)61(27)49(22)112(18)		
9	942	**	$C \geq 9$ Alkane + ?	43(100)45(31)101(23)87(19)		
10	953	**	C_6-Alkylbenzene	57(100)105(92)85(81)120(39)162(10)		
11	963	**	Aldehyde $C_8H_{16}O$	43(100)84(39)69(32)118(6)117(5)		
12	976	**	Alkyl-alcohol	43(100)57(35)71(49)132(14)		
13	980	**	?	43(100)59(51)101(28)117(10)163(3)		
14	987	**	?	69(100)87(38)45(32)41(32)95(2)111(2)126(2)		
15	995	**	Decane + ?	57(100)43(53)85(43)86(29)45(18)		
16	1008	**				
17	1019	**	C_3-Akynylbenzene	115(100)116(93)63(19)89(18)57(15)		
18	1063	***	1-Methyl-1-Phenylethanol	121(100)43(99)77(27)51(23)136(4)	Benzenemethanol	721
19	1100	**	?	99(100)155(58)81(56)127(45)109(33)82(32)		
20	1112	**	Methylindene	115(100)130(86)129(70)83(44)128(38)117(28)	1H-indene,3-methyl	323
21	1121	**	Methylindene	115(100)130(84)129(70)128(40)119(42)		
22	1164	**	Naphthalene + ?	128(100)55(62)119(42)129(16)127(13)		
23	1172	**	Chloro-?	57(100)41(38)135(15)137(5)		
24	1194	**	C_6-Alkylbenzene	91(100)119(78)134(61)43(53)162(44)83(39)		
25	1240	***	Dihydroinden-1-one	106(100)132(99)78(62)51(36)	1H-inden-1-one	710
26	1265	**	Methyltetrahydronaphthalene	131(100)146(60)117(33)103(19)91(17)63(14)51(13)147(7)	Naphthalene,1,2,3,4-tetrahydro-1-methyl	511
27	1274	**	Methyltetrahydronaphthalene	131(100)146(65)103(50)77(65)57(65)		
28	1307	**	Dimethylbenzofuran	117(100)146(90)56(50)115(42)91(25)63(22)89(17)147(11)		
29	1335	**	Mixture + #28 ?	82(100)118(83)90(72)146(44)154(36)		
30	1367	**	Mixture	[illegible]		

TABLE A-94. (Continued)

GC Peak No	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10^3
31	1362	**	Mixture ?	61(100)58(97)57(82)41(90)87(84)114(17)117(8)		
32	1376	***	Mixture ?	43(100)83(94)125(88)69(82)91(74)148(64)181(36)196(7)		
33	1381	***	Mixture ? Ketone	57(100)97(54)59(32)87(27)181(12)140(11)196(4)		
34	1427	**	Dichloro- ?	75(100)79(54)152(49)111(26)113(16)189(16)191(15)193(5)		
35	1433	**	Dichloro- ?	75(100)141(87)143(56)111(45)113(28)77(30)145(9)		
36	1447	**	Dichloro- ?	79(100)162(82)119(50)133(46)91(36)189(32)191(30)193(10)		
37	1862	**	?	57(100)56(69)85(54)135(40)209(20)211(7)		
38	1902	**	?	56(100)85(67)135(58)209(39)93(34)137(20)211(15)		
39	1902	**	?	75(100)57(60)111(48)119(46)155(41)267(17)26512)269(4)		
40	2047	**	?	57(100)75(68)101(38)87(26)173(18)247(9)		
41	2529	**	?	57(100)73(37)101(22)87(16)113(14)205(4)		

TABLE A-95. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 35E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	RI x 10^3
1	823	•	Dimethylbutanoic acid	73(100)74(92)57(78)41(51)99(20)115(4)	Butanoic acid,3,3-Dimethyl-Methyl Ester	665
2	845	••	?	43(100)85(72)102(53)69(17)115(3)		
3	857	••	Acetoxyhexanoic acid	73(100)71(74)43(74)55(46)59(31)87(20)113(16)129(4)	Hexanoic acid,5-(acetyloxy)-Methyl Ester	332
4	868	•	Methylpentanoic acid	88(100)57(35)41(30)73(7)115(6)	Pentanoic acid,2-Methyl,Methyl Ester	358
5	873	••	C ≥ 6 Fatty acid	83(100)55(77)41(38)142(14)127(6)		
6	918	••	C ≥ 6 Fatty acid	74(100)57(90)45(53)87(10)		
7	927	••	?	45(100)57(87)101(52)88(26)		
8	987	••	1-Methyl-1-phenylethanol	43(100)121(63)77(18)51(13)136(2)	Benzene methanol,α,α-Dimethyl	646
9	1020	••	Dimethylphenol	107(100)122(89)77(46)91(35)51(16)65(15)155(12)	Phenol,2,4-Dimethyl	548
10	1095	•	Allylthio-propanoic acid ME	87(100)45(98)59(86)160(68)73(63)	Propionic acid,3-(Allylthio-Methyl ester	427
11	1105	••	Methylbenzoic acid	119(100)118(84)91(79)65(35)150(37)	Benzoic acid,2-Methyl,Methyl ester	468
12	1135	••	Methylbenzoic acid	119(100)91(63)150(31)65(26)	Benzoic acid,2-Methyl,Methyl ester	451
13	1164	•••	Chloro?	57(100)87(28)135(18)89(6)137(5)		
14	1180	••	?	55(100)119(82)83(48)101(37)69(36)153(8)167(4)		
15	1208	••	Methyl-benzenepropanoic acid	119(100)91(65)77(16)103(12)178(10)51(6)65(4)		
16	1235	••	Hydroxy-methyl-benzoic acid	106(100)136(86)77(48)166(38)51(21)180(2)	Benzoic acid,2-Hydroxy-6-Methyl-Methyl Ester	663
17	1276	••	Ethenyl-benzoic acid	136(100)103(40)77(39)162(32)56(15)163(4)	Benzoic acid,4-Ethenyl-Methyl ester	606
18	1298	••	Dimethylbenzoic acid	133(100)105(40)164(28)77(26)	Benzoic acid,3,5-Dimethyl-Methyl ester	672
19	1302	••	Mixture?	172(100)97(97)113(89)157(82)125(71)79(72)59(68)		
20	1318	•••	Dimethyl-benzenepropanoic acid	119(100)91(58)135(16)77(14)65(5)165(4)192(7)		
21	1329	••	?	186(100)59(82)111(84)127(80)120(66)139(64)171(67)		
22	1335	••	?	59(100)77(56)75(55)171(44)186(55)		
23	1362	••	C_3-Alkyl-phenyl propanoic acid	119(100)91(80)77(16)79(10)51(7)206(2)		
24	1410	••	?	57(100)90(40)87(27)146(7)173(3)		
25	1469	••	Alkylbenzoic acid	115(100)174(30)89(14)63(12)		
26	1482	••	Alkylbenzoic acid	116(100)57(56)88(30)91(21)174(6)		
27	1687	••	?	87(100)85(92)55(90)59(60)186(10)		
28	1702	••	C ≥ 14 Fatty acid	87(100)102(91)		
29	1872	••	Bromo-?	135(100)75(68)99(66)177(19)247(6)245(5)		
30	2465	••	Phthalate	149(100)57(46)71(20)167(27)173(4)		

TABLE A-96. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 35E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	KI x 10^3
1	869	**	2-Propen-1-Amine N,N-Di-2-Propenyl	110(100)41(86)68(83)96(30)82(30)137(19)	2-Propen-1-amine	315
2	917	**	2,4-Hexadienal	96(100)67(73)62(66)53(59)81(40)		
3	926	**	1-Butanol 4-Butoxy	57(100)41(67)73(21)87(8)136(3)		
4	965	**	?	121(100)43(60)77(21)139(12)91(12)105(6)		
5	1030	*	Dimethylaniline	120(100)106(98)121(97)		
6	1060	**	?	156(100)132(55)106(66)79(63)127(42)141(40)		
7	1121	**	?	57(100)41(64)87(31)116(11)117(8)		
8	1136	**	Alkyl ketone	125(100)43(66)83(62)101(63)69(61)97(36)139(22)196(8)		
9	1166	**	Dihydroindene-1,2-Diol + ?	104(100)103(39)132(56)131(42)77(43)91(38)150(20)	1H-Indene-1,2-Diol	792
10	1235	**	1H Indene-1,2-Diol-2,3-Dihydro + ?	104(100)77(52)132(40)131(38)91(62)150(16)	1H-Indene-1,2-Diol	762

* Neutral compounds were so concentrated that they were also extracted into basic fraction

TABLE A-97. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 36VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.10	----	air	44(100)
2	0.14	1-10	Dichloromethane	49(100)
3	0.20	10-100	Chloroform	83(100)
4	0.26	1-10	1,1,1-Trichloroethane	97(100)99(70)61(45)117,119,121
5	0.34	10-100	Bromodichloromethane	83(100)85(65)47(23)127,129,131
6	0.58	1-10	Dibromochloromethane	129(100)127(80)131(30)79,81,206,208,210
7	1.00	~ 8	I S	75(100)110(60)

TABLE A-98. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 37VI-a

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.12	--	Air	44(100)
2	0.16	<1	Acetone	43(100)58(28)
3	0.16	~1	Diethylether	45(100)59(97)74(55)
4	0.17	10-100	Dichloromethane	49(100)84(77)
5	0.25	<1	Tetrahydrofuran	42(100)41(67)39(40)72(32)71(30)
6	0.26	<1	1,1,1 Trichloroethane	97(100)99(60)61(51)
7	0.29	<1	Benzene	78(100)
8	0.34	<1	Dichloropropane	63(100)62(75)41(60)39(42)65(32)76(30)
9	0.36	<1	Trichloroethylene	95(100)130,132(90)
10	1.00	-(8)	IS	75(100)77(33)

TABLE A-99. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 37VI-b

GC Peak No	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.086	--	Air	44(100)
2	0.12	~1	Acetone	43(100)58(30)
3	0.12	<1	Diethylether	59(100)74(80)45(65)
4	0.13	1-10	Dichloromethane	84(100)49(90)
5	0.22	<1	Tetrahydrofuran	42(100)41(65)72(33)39(31)71(29)
6	0.23	<1	1,1,1-Trichloroethane	97(100)61(70)99(62)117(12)
7	0.25	<1	Benzene	78(100)
8	0.31	<1	Dichloropropane	63(100)62(72)41(55)
9	1.00	-(8)	IS	75(100)

TABLE A-100. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 37VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.11	----	air	44(100)
2	0.14	<1	Butene	41(100)56(85)
3	0.18	<1 ea	Dimethyl sulfide + Dichloroethylene	47(100)62(85)45(70)61(50)46(45)96(8)98(4)
4	0.18	1-10	Dichloromethane	49(100)
5	0.26	<1	Tetrahydrofuran	42(100)41(42)71,72(40)
6	0.50	<1	Toluene	91(100)92(60)
7	----	<1	C_2-Alkyl benzene	91(100)106(38)
8	----	<1	C_2-Alkyl benzene	91(100)
9	----	----	I S	75(100)

TABLE A-101. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 38VI

GC Peak No	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.12	--	Air	44(100)
2	0.13	1-10	Dimethyl ether (T)	45(100)46(50)
3	0.13	~1	Butene	41(100)39(70)56(30)
4	0.16	1-10	n-pentane	43(100)42(65)41(58)39(20)57(9)72(5)
5	0.16	each 1-10	Diethyl ether + dichloroethylene	45(100)59(89)74(40)96(30)98(21)
6	0.16	20-30	Dichloromethane	49,51,84,86(100) (Sat'd.)
7	0.21	1-10	Dichloroethylene	61(100)96(70)98(42)
8	0.22	each 10-20	Chloroform + alkane	41(100)57(88)68(82)83(75)85(48)
9	0.24	~1	Tetrahydrofuran	42(100)71,72(28)
10	0.25	1-10	Dichloroethane	62(100)64(33)98(8)100(6)
11	0.26	1-10	1,1,1-Trichloroethane	97(100)99(67)61(45)117,119(18)
12	0.29	<1	Benzene	78(100)
13	0.29	<1	Carbon tetrachloride	117,119(100)47(50)35(40)82(35)
14	0.36	10-20	Trichloroethylene	95(100)130(85)132(83)97(65)
15	0.68	1-10	1,1,2,2-Tetrachloroethene	129(100)131(96)166(98)164(80)
16	0.68	1-10	Di-butoxyethane (T)	45(100)57(70)41(36)101(30)
17	0.71	1-10	Di-butoxyethane (T)	45(100)57(75)41(38)101(28)
18	1.00	-(8)	IS	75(100)77(33)
19	1.32	1-10	Dichlorobenzene	75(100)146,50(89)111(80)148(60)

TABLE A-102. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 38VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.12	--	Air	44(100)
2	0.15	~100	Acetone	43(100)58(10)
3	0.17	1-10	Dichloroethylene + Ethyl mercaptan	62(100)47(88)61(82)65(55)46(38)96(30)98(20)100(3)
4	0.18	10-100	Dichloromethane	49(100)
5	0.26	10-100	Chloroform	83(100)
6	0.29	1-10	1,2-Dichloroethane	62(100)64(33)49(20)98(10)100,102
7	0.31	~10	1,1,1-Trichloroethane	97(100)99(60)61(50)117,119,121 Sm
8	0.33	1-10	Benzene	78(100)
9	0.41	1-10	Trichloroethylene	95(100)132(98)130(96)97(65)60(43)134(30)
10	0.51	1-10	Methylisobutyl ketone	43(100)58(42)57,85(25)100(20)
11	0.57	1-10	Toluene	91(100)92(60)
12	0.70	1-10	1,1,2,2-Tetrachloroethene	166(100)164(80)129,131(73)166(50)94(50)
13	0.92	1-10	C_2 Alkyl benzene	91(100)106(60)
14	0.98	1-10	C_2 Alkyl benzene	91(100)106(63)
15	1.00	--	I.S.	75(100)
16	1.26	1-10	C_3 Alkyl benzene	91(100)106(60)
17	1.30	1-10	Dichlorobenzene	146(100)148(60)111(20)150(10)

TABLE A-103. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 39VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.10	--	Air	44(100)
2	0.10	>>100	Dimethylether	46(100)45(98)47(40)43(14)
3	0.12	10-100	Acetone	43(100)
4	0.15	10-100	Dichloromethane	49(100)
5	0.19	1-10	Chloroform	83(100)
6	0.23	<1	1,2-Dichloroethane	62(100)64(33)49(30)98,100
7	0.24	<1	1,1,1-Trichloroethane	97(100)99(67)61(55)78(38)117,119,121(8)
8	0.27	<1	Benzene	78(100)
9	0.35	<1	Trichloroethylene	95(100)130,132(90)97(60)60(58)134(33)
10	0.55	<1	Toluene	91(100)
11	0.70	<1	1,1,2,2-Tetrachloroethene	166(100)129,131(88)164(85)168(50)94(45)
12	0.93	<1	C_2-Alkyl benzene	91(100)106(30)
13	0.98	<1	C_2-Alkyl benzene	91(100)106(42)
14	1.06	<1	C_2 Alkyl benzene	91(100)106(45)
15	1.30	<1	C_2 Alkyl benzene	91(100)106(35)
16	1.31	<1	C_3-Alkyl benzene	105(100)120(28)
17	1.39	<1	C_3-Alkyl benzene	105(100)120(50)
18	1.46	1-10	Dichlorobenzene	146(100)148(67)111(33)113,150(10)

TABLE A-104. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 40VI

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.14	----	Air	44(100)
2	0.17	1-10 1-10 ea	Acetone + C_5H_{10} ea 2-Methyl-2-butene	43(100)55(50)58(32)70(20)
3	0.18	1-10 1-10 ea	2-chloropropene + 2-butanol (T)	45(100)41(68)59(50)76(10)
4	0.19	1-10	Dichloromethane	49(100)
5	0.20	<1	Isobutyraldehyde (T)	43(100)41(72)72(55)
6	0.21	<1	Unknown	43(100)44(65)45(33)67(6)68(3)
7	0.21	<1	2-Methylpropenal (T)	41(100)70(70)42(28)
8	0.23	<1	Butyraldehyde	43,44(100)41(61)57(22)72(38)
9	0.23	1-10	Methyl ethyl ketone	43(100)72(18)57(10)
10	0.25	1-10	Chloroform	83(100)85(67)
11	0.28	1-10	1,2-Dichloroethane	62(100)64(31)49(25)98(8)100(6)
12	0.29	<1	1,1,1-Trichloroethane	97(100)99(65)61(62)117,119(10)
13	0.31	<1	3-Methyl-2-butanone	43(100)41(15)86(12)
14	0.32	<1	Benzene + Unknown	78(100)41(60)57(60)58(50)
15	0.38	10-100	1,2-Dichloropropane	63(100)62(70)41(40)76(40) Sm 97,99,112,114
16	0.40	<1	Trichloethylene	95(100)130,132(90)97(60)60(50)134(30)
17	0.70	<1	1,1,2,2-Tetrachloroethene	166(100)164,129,131(90)94(60)168(58)
18	0.80	<1	Chlorobenzene	112(100)77(75)114(35)50,51(30)
19	0.97	<1	C_2 Alkyl benzene	91(100)106(40)
20	1.00	----	I.S.	75(100)

TABLE A-105. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 40VE

GC Peak No	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	--		Air	
2	--		Dichloromethane	49(100)
3	--	>100	Chloroform	
4	--	10-100	C_2 Alkyl benzene	
5	--	10-100	C_2 Alkyl benzene	
6	--	10-100	C_2 Alkyl benzene	
7	--	>100	Unknown (Saturated Spectrum)	
8	--	10-100	C_2 Alkyl benzene	
9	--	>100	Unknown (Saturated Spectrum)	

TABLE A-106. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 401

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	R.I. x 10^3
1	864	**	C ≥ 9 Alkane	43(100)166(55)165(43)129(40)131(40)133(17)168(26)170(6)		
2	859	**	Toluene	92(100)91(95)65(64)63(60)51(33)93(18)		
3	870	**	Ethylbenzene	91(100)106(28)51(12)65(12)77(10)	Benzene, ethyl	755
4	876	**	o-Xylene	91(100)106(53)105(25)77(17)65(11)107(5)	Benzene,1,2-dimethyl	632
5	891	**	p-Xylene	91(100)106(38)77(13)51(12)65(9)		
6	907	**	Nonane	43(100)57(85)41(54)85(28)71(21)99(7)128(3)		
7	951	**	C_3-Alkylbenzene	105(100)120(26)77(19)91(15)79(16)65(10)		
8	957	**	C_3-Alkylbenzene	105(100)120(44)77(15)91(12)57(9)51(8)	Benzene,1-ethyl-3-methyl	670
9	966	**	C_3-Alkylbenzene	105(100)43(32)57(31)120(29)	Benzene,(1-methyl ethyl)	361
10	982	**	C_3-Alkylbenzene	105(100)120(35)77(15)51(10)91(12)		
11	1005	**	Decane	57(100)43(90)41(49)71(40)85(26)99(7)142(4)	Decane	893
12	1008	**	C_3-Alkylbenzene	105(100)120(36)77(17)57(13)79(12)91(13)	Benzene,1-ethyl-3-methyl	603
13	1017	**	Methylstyrene	117(100)118(55)115(35)91(20)63(14)119(6)	Benzene,1-ethenyl-2-methyl	749
14	1037	**	C_4-Alkylbenzene	105(100)77(36)57(25)41(18)43(17)134(9)		
15	1053	**	C_4- Alkylbenzene	119(100)134(23)91(13)77(12)51(5)		
16	1063	**	C_4-Alkylbenzene	119(100)117(38)91(31)57(32)43(30)71(16)134(26)		
17	1067	**	C_4- Alkylbenzene	119(100)43(70)57(35)91(32)117(30)134(26)		
18	1103	**	Undecane	57(100)43(88)71(46)85(24)156(2)		
19	1119	**	C_5- Alkylbenzene	117(100)131(34)132(33)91(29)77(11)51(9)64(7)148(8)		
20	1128	**	C_5-Alkylbenzene	117(100)115(29)132(29)91(24)51(12)77(13)148(2)		
21	1157	**	Naphthalene	128(100)43(26)57(23)71(18)127(17)129(10)		

TABLE A-107. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 40E

GC Peak No	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	SI x 10^3
1	867	**	Ethylbenzene	91(100)106(28)51(13)65(12)77(10)	Benzene, ethyl	760
2	873	***	O-Xylene	91(100)106(43)77(13)51(10)65(8)63(6)	Benzene,1,2-dimethyl	729
3	888	***	P-Xylene	91(100)106(78)	Benzene,1,4-dimethyl	488
4	999	**	Chlorocyclohexanol	57(100)80(24)88(10)98(8)134(3)135(0.6)	Cyclohexanol,4-chloro,trans	561
5	1034	**	Dichlorocyclohexane	81(100)80(58)79(21)152(1)154(0.5)	Cyclohexane,1,2-dichloro	627
6	1068	**	Bromocyclohexanol	81(100)57(66)99(26)132(3)134(3)180(1)178(1)	Cyclohexanol,2-bromo	536
7	1111	**	Bromochlorocyclohexane	81(100)79(17)53(13)117(6)119(2)	Cyclohexane,1-bromo-2-chloro,cis	445
8	1551	**	Diethyl phthalate	149(100)150(12)105(8)65(8)177(17)222(0.6)	1,2-benzene dicarboxylic acid diethyl ester	650
9	1902	**	Nonadecane	57(100)43(76)71(71)85(48)99(15)113(9)127(5)	Eicosane	722
10	1979	**	Sub. Cyclohexene carboxylic acid methyl ester	134(100)107(37)57(36)79(34)167(19)166(18)234(7)	1-cyclohexene-1-carboxylic acid,4-(1,5-dimethyl-3-oxohexyl)-methyl ester	640
11	2011		Eicosane			
12	2297	**	Butylbenzyl phthalate	149(100)91(71)65(18)150(11)206(19)238(2)		
13	2497	**	Pentacosane			
14	2702	**	Heptacosane			

TABLE A-108. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 40E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	SI x 10³
1	1109	*	C ≥ 8 Fatty acid	74(100)87(46)143(4)185(3)214(1)	Undecanoic acid,10-methyl,methyl ester	518
2	1707	*	Tetradecanoic acid	74(100)87(68)43(34)55(26)143(12)157(4)211(2)	Tetradecanoic acid, methyl ester	672
3	1910	**	Hexadecanoic acid	74(64)87(68)227(2)270(1)		
4	1979	**	C ≥ 16 Fatty acid	74(100)87(73)143(20)185(7)241(3)284(2)		
5	2008	*	C ≥ 17 Fatty acid	74(100)87(74)143(16)241(3)	Heptadecanoic acid,16-methyl,methyl ester	498
6	2051	*	C ≥ 18 Fatty acid	74(100)87(75)143(20)		
7	2073	*	C ≥ 18 Fatty acid	74(100)87(80)	Heptadecanoic acid,16-methyl,methyl ester	395
8	2110	**	Octadecanoic acid	41(100)74(99)87(75)143(17)199(5)255(3)298(1)	Heptadecanoic acid,15-methyl,methyl ester	663
9	2190		C ≥ 18 Fatty acid	74(100)87(18)63(18)143(22)299(2)		
10	2307	**	C ≥ 20 Fatty acid + Phthalate	169(100)91(73)237(61)197(37)195(30)312(12)		
11	2316	**	C ≥ 20 Fatty acid	237(100)74(80)87(66)129(28)143(27)182(16)297(8)312(8)		
12	2475	**	C ≥ 21 Fatty acid	74(100)87(33)		
13	2517	**	C ≥ 22 Fatty acid	74(100)87(77)143(21)255(1.5)356(1.5)		
14	2677	*	C ≥ 23 Fatty acid	74(100)87(81)143(17)		
15	2715	*	C ≥ 24 Fatty acid	74(100)87(87)143(21)		

TABLE A-109. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 41VE

GC Peak No	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.11	--	Air	44(100)
2	0.13	>100	Dimethyl ether (T)	43-45(100) (Sat'd spectrum)
3	0.17	>100	Acetone	43(100)58(30)
4	0.18	>100	Dichloromethane	49(100)
5	0.24	1-10	Chloroform	83(100)
6	0.28	1-10	1,1,1-Trichloroethane	97(100)99(67)61(40)119(12)117(10)121(4)
7	0.91	1-10	C_2-Alkyl benzene	91(100)106(60)
8	0.98	1-10	C_2-Alkyl benzene	91(100)106(60)
9	1.00	--	I.S.	75(100)77(33)

TABLE A-110. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 42VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.14	--	Air	44(100)
2	0.18	1-10	1,1-Dichloroethylene	61(100)96(65)98(40)63(33)
3	0.19	1-10	Dichloromethane	84(100)49(95)
4	0.24	1-10	Methylethyl ketone	43(100)72(20)57(6)
5	0.26	1-10	Chloroform	83(100)
6	0.28	<1	2-Chloro-2-butene	55(100)90(35)54(33)53(25)41(18)50(13)92(11)
7	0.28	<1	Tetrahydrofuran	42(100)41(55)71,72(40)
8	0.29	<1	1,2-Dichloroethane	62(100)64(33)49(29)98(10)10(5)
9	0.30	1-10	1,1,1-Trichloroethane	97(100)99(70)61(52)117,119(8)
10	0.38	1-10	1,2-Dichloropropane	63(100)62(75)41(55)76(45)65(30)
11	0.40	10-100	Bromodichloromethane	83(100)85(65)129(10)127(8)131(2)
12	0.57	<1	Toluene	91(100)92(56)
13	0.61	10-100	Dibromochloromethane	129(100)127(82)79,81,131(25)
14	0.90	1-10	Bromoform	173(100)171(60)175(48)79,81(35)252,254(5)
15	1.00	--	I.S.	75(100)

TABLE A-111. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 43VI

GC Peak No	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.13	----	air	44(100)
2	0.18	10-100	Dichloromethane	49(100)
3	0.52	<1	methyl isobutyl Ketone	43(100)58(30)85(16)100(9) (also seen in previous run)
4	0.81	----	Chlorobenzene	112(100)77(72)50,51,114(32)
5	0.98	----	C_2 alkyl benzene	91(100)106(60)
6	1.00	----	I S	75(100)

TABLE A-112. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 43VE

GC Peak No	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.13	--	Air	
2	0.18	1-10	Dichloromethane	49(100)
3	0.28	1-10	1,1,1-Trichloroethane	97(100)99(67)61(50)
4	0.31	1-10	Benzene	78(100)
5	0.49	1-10	Methyl isobutyl ketone	58(100)43(99)57(57)41(46)85(43)100(30)
6	0.55	<1	Toluene	91(100)92(53)
7	0.59	1-10	n-Butyl acetate	43(100)56(25)73(12)
8	0.91	1-10	C_2-Alkyl benzene	91(100)106(47)
9	0.97	1-10	C_2-Alkyl benzene	91(100)106(45)
10	1.00	--	I.S.	75(100)110(35)

TABLE A-113. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 43I

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10^3
1	844	**	Dichloro C_4-Alkene	41(100)55(83)90(63)77(43)92(17)124(4)126(3)		
2	855	*	Chlorohexane	91(100)55(80)93(33)41(63)	Hexane, 1-Chloro-	686
3	915	**	Chloromethylbutene	55(100)69(68)68(56)41(30)91(31)93(9)104(4)106(2)	1-Butene, 2-(Chloromethyl)-	358
4	1010	**	?	69(100)41(52)82(24)67(20)90(8)105(4)118(2)		
5	1056	*	Chloroethenylbenzene	89(100)125(95)53(70)63(41)91(33)127(60)138(4)140(2)		
6	1630	**	Benzenesulfonamide N,4-Dimethyl	91(100)65(29)121(23)150(26)92(20)185(27)186(3)	Benzenesulfonamide, N-4-Dimethyl	595
7	2110	*	C ≥ 18 Fatty Acid	74(100)87(80)143(23)298(3)	Heptadecanoic Acid, 16-Methyl-, Methyl	560
					Ester	
8	2321	*	C ≥ 20 Fatty Acid	87(100)55(100)97(64)197(83)200(23)229(8)	Octadecanoic Acid, 12-Hydroxy-, Methyl	601
					Ester	

TABLE A-114. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 43E

GC Peak No	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10^3
1	974	***	Phenol	94(100)66(48)65(26)95(4)		
2	1042	**	Methylphenol	108(100)107(94)79(46)77(44)		
3	1064	***	Methylphenol	41(100)107(80)77(25)79(10)109(5)		
4	1137	**	Dimethylphenol	107(100)122(76)121(40)77(36)79(22)91(27)	Phenol,3,4-Dimethyl	537
5	1162	**	Dimethylphenol	107(100)122(82)77(33)79(21)91(22)	Phenol,2,5-Dimethyl	542
6	1399	*	C > 10 Fatty acid	74(100)87(67)143(13)171(9)	Decanoic acid,8-Methyl, Methyl ester	457
7	1708	*	C ≥ 12 Fatty acid	74(100)87(74)143(20)199(12)	Undecanoic acid,11-Bromo, Methyl ester	489
8	2080	*	C ≥ 17 Fatty acid	74(57)87(35)264(6)	10-Undecenoic acid, methyl ester	478
9	2110	*	C ≥ 18 Fatty acid	74(100)87(70)143(15)199(6)255(4)	Triacontanoic acid, methyl ester	356

TABLE A-115. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 44VE

GC Peak No	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.14	--	Air	44(100)
2	0.18	10-100	Acetone	43(100)58(30)
3	0.19	10-100	Dichloromethane	84(100)49(73)86(62)
4	0.23	1-10	Methylethyl ketone	43(100)72(20)
5	0.32	1-10	Benzene	78(100)
6	0.57	1-10	Toluene	91(100)92(55)
7	1.00	8	I.S.	75(100)77(33)

TABLE A-116. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 44E

GC Peak No	Retention Index	Amount, μg?	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	SI x 10^3
1	970	***	Phenol	94(100)66(46)65(25)95(7)93(4)		
2	1038	***	Methylphenol	108(100)107(92)79(38)77(37)51(15)63(9)90(8)89(16)91(7)		
3	1062	***	C_2-Alkylphenol	107(100)108(75)77(38)79(34)122(19)51(13)53(11)	Phenol,2-Methyl	370
5	1125	**	C_2-Alkylphenol	107(100)122(42)77(33)79(17)51(9)63(8)65(7)123(4)		
6	1131	***	C_2-Alkylphenol	107(100)122(81)121(67)77(28)91(25)79(19)51(9)123(6)		
7	1156	***	C_2-Alkylphenol	107(100)122(40)77(22)91(9)79(7)65(6)51(7)123(7)138(2)		
8	1182	**	C_3-Alkylphenol	107(100)122(92)121(71)77(42)91(29)136(5)		
9	1212	**	C_3-Alkylphenol	121(100)136(61)91(31)77(26)167(15)65(8)51(8)		
10	1222	**	C_3-Alkylphenol	121(100)136(27)91(17)77(15)65(5)51(4)103(4)107(4)	Phenol,3-Ethyl-5-Methyl	673
11	1265	**	C_3-Alkylphenol	171(100)136(61)107(61)77(27)91(24)65(7)53(5)		
12	1253	**	C_3-Alkylphenol	121(100)136(67)91(38)77(24)107(16)79(10)65(8)53(8)		
13	1268	*	C_4-Alkylphenol	121(100)136(35)91(23)77(20)107(15)65(8)51(7)		
14	1321	**	C_4-Alkylphenol	133(100)136(90)135(59)105(40)91(63)77(68)51(21)65(17)		
15	1330	**	C_6-Alkylphenol	133(100)134(53)135(27)105(33)77(27)91(20)150(20)51(20)	-	
16	1343	*	Methylallylphenol	133(100)107(90)168*40)77(35)63(14)51(16)162(5)		
17	1370	**	C_4-Alkenylphenol + ?	133(100)148(34)105(26)77(13)91(9)51(7)63(7)	Phenol,2-(2-methyl-2-propenyl)	693
18	1389	*	C_4-Alkylphenol	133(100)148(57)105(22)91(22)77(17)63(13)149(12)		
19	1426	**	C_4-Alkylphenol + ?	133(100)167(61)148(55)91(19)105(18)77(14)51(10)162(7)166(1)		
4	1083	**	Benzoic Acid	105(100)77(60)136(40)51(28)		

TABLE A-117. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 45VI

GC Peak No.	Relative Retention Time	Amount, μg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.12	--	Air	44(100)
2	0.16	<1	Diethylether	45(100)59(95)74(50)
3	0.16	~10	Dichloromethane	49(100)84(37)51(28)
4	0.32	<1	Chloroform	83(100)85(67)
5	0.24	<1	Tetrahydrofuran	42(100)41(77)71,72(33)
6	0.26	<<1	1,1,1-Trichloroethane	97(100)99(65)
7	0.28	<1	Benzene	78(100)
8	0.35	<1	Trichloroethylene	95(100)132(80)130(78)
9	0.67	~10	1,1,2,2-Tetrachloroethene	166(100)129(90)131(85)
10	1.00	-(8)	IS	75(100)77(33)

TABLE A-118. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 45VE

GC Peak No	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.11	----	Air	44(100)
2	0.12	10-100	Butene	56(100)41(98)
3	0.17	10-100	Chloromethyl propene	72(100)55(82)63(78)90(40)92(12)72 + unknown
4	0.22	>100	Chloromethyl propene	90(100)54(95)55(90)
5	0.32	10-100	Benzene	78(100)
6	0.36	>100	Dibromomethane	93(100)174(90)95(85)172(50)79,81(25)
6	0.36	>100	Dibromomethane	93(100)174(90)95(85)172(50)79,81(25)
7	0.49	10-100	Unknown	93(100)91(72)77(58)108(33)
8	0.51	10-100	$C_4H_8C_{12}$ eg 1,3-dichloro-2-methyl propane	77(100)55(80)79(70)41(60)91(35)75(30)49(25)76(20)93(10)111(8)113(5)
9	0.56	>100	Toluene	91(100)92(65)
10	0.60	>100	Unknown	65(100)51(60)63(58)50(42)62(25)89(25)93(20)45(20)
11	0.67	1-10	Unknown	66(100)55(90)90(72)65(50)75(28)
12	0.69	1-10	Unknown	55(100)67(70)95(60)68(60)53(28)41(25)81(15)
13	0.69	1-10	Unknown	55(100)41(85)77(80)54(45)76(40)90(28)
14	0.71	1-10	C_8H_{14}, eg 3,4-dimethyl-2,4-hexadiene	95(100)67(80)55(34)41(30)110(28)
15	0.72	1-10	C_8H_{14} + Unknown	95(100)93(80)91(68)67(60)77(48)55(42)108(40)110(26)
16	0.75	1-10	C_8H_{14} + Tetrachloroethene	95(100)67(40)110(28)93(25) Small 129,131,164,166,168
17	0.82	>100	$C_4H_6Cl_2$	89(100)53(98)124(50)91(48)126(33)50(30)
18	0.86	>100	1,3-Dichloro-2-methylenepropane	88(100)89(65)53(60)90(50)69(38)
19	0.93	10-100	C_8H_{12}	93(100)91(90)77(60)108(60)79(18)
20	0.94	10-100	Unknown	55(100)60(70)116(70)87(50)
21	0.95	10-100	C_2 Alkyl benzene	91(100)106(33)
22	0.96	10-100	Unknown	93(100)91(55)108(50)77(50)55(40) on 171,173,175
23	0.98	10-100	C_8H_{10}	106(100)105(60)91(45)77(28)56(22)
24	0.99	10-100	Unknown	101(100)55(66)73(53)43(35)
25	1.01	10-100	C_8H_{14}	67(100)95(95)110(90)55(38)41(30)
26	1.02	10-100	Unknown	77(100)79(30)70(28)41(26)175(12)177(8)
27	1.05	10-100	C_2-Alkyl benzene	91(100)106(40)
28	1.06	10-100	Unknown	77(100)93(100)91(95)108(55)75(50)126(8)
29	[illegible]	10-100	Unknown	53(100)89(70)88([illegible])

TABLE A-118. (Continued)

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
30	1.10	10-100	Diethyl disulfide	122(100)66(82)94(50)124(8)
31	1.17	>100	Unknown	113(100)75(100)111(95)58(66)49(54)124(15)
32	1.32	10-100	Unknown	109(100)67(60)41(24)77(22)91(21)
33	1.35	10-100	Unknown	109(100)55(98)53(72)67(65)142(M)
34	1.52	10-100	C_5 alkyl benzene	133(100)105(70)148(55)77(22)
35	1.54	10-100	1 Hindene $C_{11}H_{12}$ M146 2,3-dihydre-1,3-dimethyl	131(100)91,119,146(40)
36	1.56	10-100	$C_{11}H_{14}$, eg methyl butenyl benzene	131(100)91(42)146(40)105(30)77(22)
37	1.58	10-100	$C_{11}H_{16}$	131(100)91(53)146(50)105(30)
38	1.61	>100	Unknown	121(100)93(95)97(90)65(90)115(60)109(50)198(30)
39	1.65	10-100	$C_{11}H_{14}$, eg 1,1-dimethyl-2-propenyl benzene	131(100)91(62)146(50)115(38)
40	1.66	10-100	Unknown	55(100)91(50)90(25)93(23)143(18)158(8)
41	1.67	10-100	2,3-di hydro-4,7-dimethyl 1 H-Indene $C_{11}H_{14}$ M146	131(100)146(70)91(42)115(30)
42	1.73	10-100	4-(2-butenyl)-1,2-dimethyl benzene $C_{12}H_{16}$ M160	145(100)91(88)160(40)55(55)
43	1.95	10-100	1-(2-butenyl)-2,3-dimethyl benzene $C_{12}H_{16}$ M160	145(100)105(40)125(30)124(30) (no 160)

TABLE A-119. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 45E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable [illegible] Match	
					Compound	E.I. $\times 10^3$
1	873	***	$C_4H_6Cl_2$	89(100)53(99)91(35)124(31)126(20)		
2	877	**	$C_4H_6Cl_2$ Dichlorobutene	88(100)89(89)53(96)90(38)124(16)126(9)128(1)		
3	883	**	Methylpentanone	41(100)85(55)63(55)65(18)57(16)	2-Pentanone,4-methyl	458
4	891	**	Xylene + ?	55(90)73(78)91(56)106(21)		
5	905	**	2-Propenal-3(2-furanyl)	71(100)66(76)122(65)43(50)96(46)126(6)		
6	933	***	Chloro-alkene	111(100)75(81)113(66)77(25)89(23)124(9)126(6)		
7	950	**	?	43(100)99(76)55(58)70(35)100(4)		
8	1003	**	Chloro-alkene	41(100)43(60)85(30)57(16)87(5)99(0.6)97(0.4)		
9	1037	**	Acetophenone	105(100)77(88)51(36)120(26)	Ethanone,1-phenyl	719
10	1069	**	1-Methyl-1-phenylethanol	79(100)107(76)77(57)122(22)51(26)	Benzene methanol,α-methyl	637
11	1095	***	C_3-alkylbenzene	133(100)105(70)148(57)77(19)91(20)51(19)63(12)	Benzene,1-ethyl-3-(1-methyl ethyl)	480
12	1115	**	?	61(100)154(70)94(33)122(16)156(8)		
13	1163	***	Mixture + Benzene,1,1'oxybis[4-methyl]	97(99)121(92)65(94)93(93)81(67)170(17)198(100)199(8)		
14	1176	***	Ethanol,1-(2-butoxyethoxy)	45(100)57(80)75(17)87(10)89(8)132(1)	Ethanol,1-(2-butoxy ethoxy)	817
15	1194	**	3(2H)-Benzofuranone, dimethyl	94(100)162(56)76(38)104(36)43(33)121(28)147(22)		
16	1208	**	?	75(100)111(65)99(48)157(42)50(18)127(22)159(14)		
17	1231	**	Benzoic acid,2-propenyl ester	105(100)77(42)51(20)117(3)162(2)	Benzoic acid,2-propenyl ester	584
18	1255	**	3(2H)-Benzofuranone dimethyl	162(100)104(78)77(69)51(52)131(54)78(44)135(38)163(13)	3(2H)-Benzofuranone dimethyl	520
19	1264	**	?	111(100)97(98)81(92)65(72)138(67)170(33)200(32)198(18)202(2)		
20	1273	**	p-Methoxypropiophenone	135(100)77(27)164(22)51(16)105(10)79(9)		
21	1325	***	Phosphorodithioic acid,o,o-diethyl S-ethyl ester	186(100)97(76)121(61)65(56)93(57)125(25)214(24)		
22	1373	**	$C_{14}H_{18}O$	202(100)187(50)145(67)159(60)91(48)203(16)	Benzene,1-(5,5-dimethyl-1-cyclopenten-1-yl)2-methoxy	32
23	1395	**	?	86(100)81(98)111(82)55(77)135(76)163(47)191(52)224(37)		
24	1452	**	Mixture +	176(100)131(98)77(91)51(82)146(84)193(72)115(65)91(66)		
25	1473	***	Homolog of #21	97(100)121(93)65(76)93(71)125(64)153(49)129(44)240(50)		
26	1505	***	C_8-Alkenylphenol	107(100)135(96)		
27	1529	***	?	55(100)123(98)106(35)63(29)124(8)193(1)		
28	1582	***	Alkyl-tetrahydronaphthalene-1,1-dioxide	146(100)176(99)131(92)193(88)77(66)51(58)91(46)218(5)		
29	1603	**	1,2-Benzisothiazole,3-ethoxy	196(100)76(56)77(52)106(37)120(28)147(21)169(17)211(14)	1,2-Benzisothiazole,3-ethoxyl,1,-dioxide	682
30	1613	**	" Isomer of #29	97(100)65(76)93(52)174(42)202(46)238(24)322(16)		

TABLE A-119. (Continued)

GC Peak No	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10^3
31	1715	***	Di-2-propenyl phthalate	149(100)41(52)104(46)76(44)132(37)189(49)190(6)	1,2-Benzenedicarboxylic acid,di-2-propenyl ester	491
32	1788	***	Subst.-benzofuranone	189(100)190(13)76(18)115(16)41(18)149(11)		
33	2121	**	?	199(100)103(80)76(39)135(38)61(24)162(23)		
34	2240	**	Sulfur-containing?	97(100)65(62)93(62)121(62)125(48)180(49)332(21)243(17)299(8)		
35	2379	***	?	176(100)177(31)57(21)149(22)119(14)91(10)193(6)		
36	2611	**	Phthalate	149(100)		

TABLE A-120. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 45E

GC Peak No	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10^3
1	876	**	Trimethylpiperidine	112(100)86(98)55(37)127(26)	Piperidine, 1,2,6-Trimethyl-	434
2	882	**	Mixture ?	41(100)85(71)43(52)57(18)	2-Hexanone, 3,4-Epoxy-	501
3	911	**	C_4-Alkylpiperidine MW 141	71(100)126(94)41(59)100(23)141(11)		
4	976	**	Methylpyridine + ?	93(100)65(38)65(18)92(12)140(8)155(1)		
5	1056	*	Methylaniline	106(100)107(76)122(1)77(20)91(5)		
6	1178	**	Methoxyaniline MW 123	80(100)108(79)123(56)53(22)65(13)		
7	1344	**	Pentamethylaminobenzene MW 163	148(100)163(98)121(52)131(26)103(24)93(22)77(20)		

TABLE A-121. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 46VI

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.12	--	Air	44(100)
2	0.16	>100	Dichloromethane	49(100)84(100) Sat'd.
3	0.22	1-10	Chloroform	83(100)85(65)
4	0.25	1-10	Dichloroethane	62(100)64(33)98(15)
5	0.26	1-10	1,1,1-Trichloroethane	97(100)61(70)99(67)117(15)
6	0.34	10-100	Dichloropropane	63(100)62(70)41(50)39(35)65(30)76(23)
7	0.36	~1	Trichloroethylene	95(100)130(80)132(79)97(63)60(45)
8	0.54	1-10	Toluene	91(100)92(60)
9	0.68	<1	Tetrachloroethene	131(100)166(95)129(80)164(73)94(61)47(48)
10	1.00	-(8)	IS	75(100)77(33)

TABLE A-122. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 46VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.13	--	Air	44(100)
2	.18	1-10	Dichloromethane	84(100)86(70)49(50)
3	.29	1-10	1,1,1-Trichloroethane	97(100)99(70)61(25)117(18)

TABLE A-123. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 47VI

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.11	----	air	44(100)
2	0.17	1-100	acetone	43(100)
3	0.18	10-100	Dichloromethane	49(100)
4	0.23	<1	Dichloroethylene *	61(100)96(72)98(50)63(30)
5	0.24	1-10	isopropyl ether	45(100)43(50)41(15)87(12)
6	0.30	<1	benzene *	78(100)
			*Probably in blank	

TABLE A-124. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 47VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.14	--	Air	44(100)
2	.19	1-10	Diethylether	45(100)59(96)74(50)
3	.20	10-100	Dichloromethane	49(100)86(50)
4	.25	1-10	1,1-Dichloroethylene	61(100)96(45)
5	.27	1-10	Isopropyl ether	45(100)45(43)87(20)
6	.29	.1-1	Tetrahydrofuran	42(100)72(30)71(28)
7	.34	.1-1	Benzene	78(100)
8	.65	.1-1	Dichloropropane	76(100)41(67)78(40)
9	1.00	(8)-	I.S.	75(100)77(30)110(28)

TABLE A-125. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 48VI

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.11	----	Air	44(100)
2	0.21	10-100	Dichloromethane	49(100)
3	0.21	1-10	Cyclopentadiene	66(100)65(65)
4	0.26	<1	Dichloroethylene	61(100)96(52)63,98(33)
5	0.27	<1	Chloroform	83(100)47(80)85(60)
6	0.31	~1	1,1,1-trichloroethane	97(100)99(63)61(50)63(18)117,119(8)121(4)
7	0.41	~1	trichloroethylene	130(100)132(97)94(94)96(62)
8	0.52	<1	methylisobutyl Ketone	43(100)58(30)85(15)100(10)
9	0.58	<1	toluene	91(100)
10	0.71	<1	1,1,2,2-tetrachloroethene	166(100)129(90)
11	1.00	----	I S	75(100)

TABLE A-126. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 48VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.11	----	air	44(100)
2	0.18	10-100	Dichloromethane	84(100)
3	0.31	1-10	1,1,1-trichloroethane	97(100)99(70)61(25)119(10)117(8)121(4)
4	1.00	----	I S	75(100)

TABLE A-127. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 49VI

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.13	---	Air	44(100)
2	0.16	>100	Acetone	43(100)58(40)
3	0.17	10-100	C_5H_{10}, eg 2-Me-2-butene	55(100)70(28)41,42(20)
4	0.17	10-100	Diethyl ether (T) Sat'd	45,59,74(100)
5	0.17	10-100	Dichloromethane	49(100)
6	0.18	10-100	Carbon disulfide	76(100)
7	0.22	10-100	Dichloroethylene	61(100)96(60)98(40)63(35)
8	0.24	10-100	Chloroform	83(100)
9	0.28	<1	1,1,1-Trichloroethane	97(100)99(67)61(55)117,119(12)
10	0.28	1-10	2-Methyl-2-butanol	59(100)73(57)43(46)55(45)
11	0.30		Benzene	78(100)
12	0.31	10-100	Carbon tetrachloride	119(100)117(80)47(50)82(48)
13	0.34	1-10	Cyclohexene	67(100)54(70)82(40)41(25)
14	0.38	10-100	Trichloroethylene	95(100)130(82)132(79)60(62)
15	0.59	10-100	Toluene	91(100)92(60)
16	0.75	1-10	1,1,2,2-Tetrachloroethene	166(100)129,131(90)164(82)166(50)89(42)
17	0.84	1-10	Chlorobenzene	112(100)77(58)114(33)
18	0.90	1-10	C_2- Alkyl benzene	91(100)106(30)
19	0.93	10-100	C_2- Alkyl benzene	91(100)106(50)
20	0.97	1-10	Cyclooctatetraene	104(100)78(62)103(60)
21	0.98	1-10	C_2 Alkyl benzene	91(100)106(40)
22	1.00	----	I.S.	75(100)
23	1.05	1-10	Bromobenzene	156(100)158(98)77(75)
24	1.17	1-10	Butyl Ketone	85(100)57(88)41(35)142(20)127(10)

TABLE A-128. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 49VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.10	----	air	44(100)
2	0.13	>>>100	Diethyl ether	59(100)45(78)74(70)
3	0.15	10-100	Dichloromethane	49(100)
4	0.20	10-100	Chloroform	83(100)
5	0.22	>100	Tetrahydrofuran	42(100)41(55)71(50)72(50)
6	1.00	----	I S	75(100)
7	1.15	1-10	$C_{10}H_{16}$	93(100)91(58)92(45)77(30)79(25)105(20)121(15)

TABLE A-129. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 49I

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10^3
1	862	**	Oxybicyclo[4.1.0]heptane	83(100)41(62)55(40)54(40)69(30)97(13)	7-Oxabicyclo[4.1.0]heptane	586
2	868	**	Ethylbenzene	91(100)106(41)77(15)51(12)65(9)	Benzene, ethyl	779
3	873	**	C_2-Alkylbenzene + Alkyl alcohol	56(100)55(56)43(56)69(29)91(8)106(3)105(1)	1-Pentanol	635
4	1061	**	Ethane,1,1'-oxybis[2-ethoxy]	45(100)59(44)72(43)73(40)103(4)	Ethane,1,1'-oxybis[2-ethoxy]	577
5	1130	**	Dibromocyclohexane + ?	81(100)79(85)53(60)41(43)77(25)97(23)132(1)		
6	1165	**	Bromocyclohexanol	81(100)99(30)57(26)55(22)79(19)127(5)128(2)	Cyclohexanol,2-bromo	418
7	1209	**	Dibromocyclohexane	81(100)79(20)53(14)41(12)117(10)127(4)119(3)		
8	1529	**	1,1'-Bicyclohexyl-ethyl	83(100)55(64)111(32)41(28)67(10)196(8)	1,1'-Bicyclohexyl-2-ethyl-trans	306
9	1567	***	Subst.-cyclohexane	95(100)55(80)113(62)41(58)67(46)112(29)83(26)114(5)178(1)		
10	1677	*	? Isomer of #9	95(100)55(56)67(35)41(34)96(35)97(30)178(16)		
11	1705	**	N-4-ethoxyphenylacetamide	108(100)109(92)179(40)137(36)80(25)81(20)43(35)	Acetamide,N-(4-ethoxyphenyl)	814
12	2511	**	Bis(2-ethylhexyl)phthalate	149(100)167(29)57(34)70(22)71(22)		

TABLE A-130. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 49I

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	K.I. x 10³
1	1637	**	Benzenesulfonic acid,4-methyl hydrazide	91(100)155(59)65(48)186(59)187(4)		
2	1509	*	C ≥ 12 Fatty acid	74(100)87(66)		
3	1625	**	Isomer of #1	91(100)65(39)121(32)155(25)185(27)186(2)		
4	1709	*	C ≥ 14 Fatty acid	74(100)87(75)		
5	1737	*	Methyl benzenesulfonamide	91(100)171(52)155(50)107(48)65(38)	Benzenesulfonamide,4-Methyl	578
6	1884	*	C ≥ 15 Fatty acid		10-Undecenoic acid, methyl ester	616

TABLE A-131. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 49E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	K.I. x 10³
1	883	**	Chlorobenzene	112(100)77(79)114(31)51(31)50(30)78(5)	Benzene, chloro	382
2	932	*	Methylcyclohexanone	83(100)42(66)41(66)54(66)55(43)69(30)97(12)	Cyclohexanone,4-methyl	399
3	960	*	Chlorocyclohexane	67(100)87(42)55(36)41(35)54(33)118(1)120(0.3)	Cyclohexane, chloro	584
4	999	*	Decane	57(100)43(91)71(36)85(22)99(5)142(3)	Decane	889
5	1009	**	Chlorocyclohexanol	57(100)80(26)81(18)41(18)88(12)98(9)134(4)136(1)	Cyclohexanol,4-chloro	367
6	1015	**	Subst.-ketone	43(100)81(50)71(41)108(33)111(30)139(18)154(18)	2-Oxabicyclo[2,2,2]octane,1,3,3-trimethyl	707
7	1061	**	?	45(100)59(43)72(40)73(38)123(10)		
8	1079	**	C_5-Alkenylcyclopentane	81(100)87(68)88(55)89(50)110(47)95(40)124(4)152(3)	Cyclopentane,2-ethylidene-1,1-dimethyl	558
9	1099	*	Undecane	57(100)43(93)71(46)85(22)156(2)	Dodecane	772
10	1130	**	Alkyl-cyclohexene	81(100)79(80)53(60)77(58)105(39)51(34)148(2)	Cyclohexene,3-(2-propynyl)	408
11	1181	***	Iodoheptane	81(100)99(50)57(40)55(36)79(30)127(8)128(4)226(2)		
12	1229	***	Mixture + Iodochlorocyclohexane	53(100)67(99)81(97)117(28)127(15)244(8)246(3)		
13	1348	*	1,1'-biphenyl	154(100)153(40)152(27)115(21)76(17)51(16)63(14)		
14	1364	**	?	77(104)107(67)51(36)137(24)152(20)		
15	1433	*	Bromonaphthalene	127(100)126(28)63(22)206(74)207(71)	Naphthalene,1-bromo	575
16	1521	*	1,1'-Bicyclohexyl-2-ethyl	83(100)55(50)111(26)41(20)194(5)	1,1'-Bicyclohexyl,2-ethyl-,trans	308
17	1533	*	Mixture ? + isomer of #8	83(100)55(86)112(55)41(50)109(38)165(32)203(4)		
18	1615	**	?	83(100)55(86)165(58)95(59)41(49)109(42)		
19	2093	**	?	93(100)188(56)271(2)		

TABLE A-132. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 49E

GC Peak No	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	SI x 10^3
1	1416	*	Imidazolidine, C_2 Alkylphenyl	85(100)57(67)56(61)91(36)117(17)		
					Morpholine, 3,4-DiMethyl-2-Phenyl- (2R, Trans-)	361
2	1432	*	Imidazolidine, C_3 Alkylphenyl	99(100)70(64)162(58)91(42)71(40)117(12)190(14)		
3	1480	**	?	100(100)77(22)44(15)72(14)182(6)167(3)		
4	1545	**	Isomer of #3	100(100)72(66)77(39)44(50)56(21)180(10)		
5	1913	**	?	58(100)71(58)167(19)180(14)182(8)183(4)184(0,2)		

TABLE A-133. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 50VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.14	----	Air	44(100)
2	0.18	1-10	Dichloromethane	49(100)
3	0.24	<1	Chloroform	83(100)
4	0.36	<1	1,2-dichloropropane	63(100)62(70)41(55)71(50)65(30) Sm 97,99,112,114
5	0.64	1-10	1,2,2-trichloropropane	97(100)99,111(70)113(45) Sm 131,133,135
6	1.00	——	I S	75(100)
7	1.20	<1	C_3 alkyl benzene	105(100)120(45)
8	1.21	<1	dichlorobenzene	146(100)148(70)111(33)75(25)
9	1.24	<1	C_3 alkyl benzene	105(100)120(50)
10	1.35	<1	C_4 alkyl benzene	119(100)134(30)
11	1.41	<1	C_4 alkyl benzene	119(100)134(30)
12	1.41	<1	C_4 alkyl benzene	119(100)134(40)
13	1.44	<1	$C_{10}H_{12}$ eg C_2 styrene	117(100)132(40)115(38)133(28)
14	1.45	<1	C_4 alkyl benzene	119(100)134(40)
15	1.48	1-10	trichlorobenzene	180(100)182(95)184(40)145(25)147(15)

TABLE A-134. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 50E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10^3
1	835	**	1,1-Dioxolane-2-(chloromethyl)	73(100)45(46)121(16)97(6)123(5)	1,3-Dioxolane,2-(chloromethyl)	343
2	1003	**	2-Propanol,1-(2-methoxy-1-methylethoxy)	59(100)45(60)103(28)73(28)104(4)	2-Propanol,1-(2-methoxy-1-methylethoxy)	711
3	1007	**	" Isomer of #2	59(100)45(62)73(28)103(26)	"	672
4	1215	***	Benzenemethanamine,N-methyl,N-nitroso	91(100)120(63)92(48)150(28)65(20)51(10)151(3)	Benzenemethanamine,N-methyl-N-nitroso	374
5	1360	**	Nitroaniline	65(100)138(83)92(58)80(30)52(24)118(26)139(6)121(6)	Benzenenamine,3-nitro	373
6	1501	**	Chloroalkylsubst. -phenol	108(100)91(46)107(36)65(22)200(16)202(5)		
7	1658	**	2,4-Bis(1-methylbutyl)-phenol	205(100)71(26)43(24)206(16)234(6)	Phenol,2,4-bis(1-methyl butyl)-	433
8	1674	**	C ≥ 16 Alkane	57(100)43(70)41(42)76(59)85(47)99(14)148(4)	Pentacosane	646
9	1700	***	?	44(100)68(83)201(78)186([illegible]7)173(46)96(40)203(26)214(6)		
10	2337	**	?	91(100)117(24)65(12)155(5)167(4)207(6)208(5)		
11	2511	**	Bis(2-ethylhexyl)phthalate	169(100)57(44)71(28)167(28)113(10)	1,2-Benzenedicarboxylic acid, diisopropyl ester	368

TABLE A-135. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 50E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	RI x 10^3
1	1268	*	Hydroxybenzeneacetic acid	77(100)107(95)161(84)56(34)79(38)162(8)	Benzeneacetic acid,α-hydroxy-methyl ester	515
2	1299	*	Trichlorophenol	195(100)197(96)199(30)167(76)169(72)210(50)212(46)214(15)	Benzene,1,3,5-Trichloro-2-methoxy	786
3	1341	**	Benzenedicarboxylic acid monomethyl este	41(100)91(45)180(41)107(30)121(29)77(16)65(13)181(2)		
4	1361	*	Trimethylbenzoic acid	167(100)146(64)178(37)119(36)91(34)163(13)	Benzoic acid,2,4,5-Trimethyl-methyl ester	617
5	1364	**	Trimethylbenzoic acid	147(100)146(81)119(55)91(53)178(52)77(25)179(6)	Benzoic acid,2,4,5-Trimethyl-methyl ester	560
6	1554	*	Hydroxy-trimethylbenzoic acid	105(100)133(79)134(56)77(50)164(60)196(40)195(4)		
7	1567	**	Chloro- ?	113(100)161(93)151(91)77(70)217(92)219(19)		
8	1628	**	Dichloro- ?	126(100)154(66)95(54)188(64)190(41)253(36)255(25)257(4)		
9	1705	**	Bromo- ?	246(100)248(100)75(81)62(72)276(42)278(42)		
10	1073	**	?	205(100)57(59)91(43)175(64)177(54)217(29)261(6)271(3)		
11	1906	***	?	41(100)147(64)161(16)277(35)292(16)219(15)293(2)		
12	2333	**	Chloro- ?	101(100)77(66)79(29)262(13)264(4)326(8)328(4)		
13	2399	**	Chloro- ?	106(100)77(78)90(48)126(24)296(16)197(14)232(12)298(6)		
14	2475	**	Chloro- ?	65(100)92(96)90(87)126(88)282(65)284(23)217(19)		

TABLE A-136. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 50E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	RI x 10^3
1	977	***	Methylpyridine	93(100)66(100)56(60)92(40)94(23)63(18)52(16)	Pyridine, 3-Methyl	484
2	1067	**	Methylaniline	106(100)107(89)77(22)70(18)51(10)	Benzenamine, 4-Methyl	626
3	1167	*	C_6-Alkylpyridine	120(100)77(30)130(22)51(12)	1,2-Ethanediamine, N,N'-DiMethyl-N,N'-	323
					diphenyl-	
4	1163	***	2-Methoxyaniline	80(100)108(80)123(53)53(18)	Benzenamine, 2-Methoxy	706
5	1182	*	3-Methyl-5-Ethoxypyrazole	98(100)97(40)126(32)67(22)		
6	1195	**	Benzeneacetamide, N-(Aminocarbonyl)	118(100)91(36)134(32)116(26)65(15)178(16)179(2)	Benzeneacetamide, N-(Aminocarbonyl)-	228

TABLE A-137. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 51VI

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.13	--	Air	44(100)
2	0.17	1-10	Diethylether	59(100)45(98)74(58)
3	0.18	10-20	Dichloromethane	49(100)84(40)
4	0.24	∿1	Chloroform	83(100)85(67)
5	0.25	1-10	1,1-di-propoxyethane (T)	45(100)43(45)87(22)59(15)95(6)
6	0.27	<1	Tetrahydrofuran	42(100)71,72(33)
7	0.28	1-10	Dichloroethane	62(100)49(38)64(33)98(12)
8	0.29	1-10	1,1,1-Trichloroethane	97(100)99(67)61(55)63(18)117,119(14)
9	0.38	80-100	Dichloropropane	63(100)62(70)41(50)65(30)76(28) Sm 112,114
10	0.40	∿1	Trichloroethylene	95(100)130(78)132(76)97(63)134(33)
11	0.75	1-10	1,1,2,2-Tetrachloroethene	166(100)129(89)131(88)164(82)
12	1.00	-(8)	IS	75(100)77(33)

TABLE A-138. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 51VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.12	--	Air	44(100)
2	0.16	1-10	Chloropropene + Diethyl ether	74(100)59(85)41(78)39(65)45(30)76(27)78(10)
3	0.16	10-100	Dichloromethane	84(100)49(99)86(95)
4	0.19	<1	Methylpentane	43(100)42(55)41(33)71(22)86(2)
5	0.20	<1	C_6H_{14}	57(100)41(82)56(78)43(53)72(9)86(4)
6	0.22	1-10	Chloroform	83(100)85(67)47(55)
7	0.24	<1	Tetrahydrofuran	42(100)41(80)39(45)55(38)72(35)71(34)
8	0.25	1-10	Dichloroethane	62(100)49(50)64(33)98(8)100(6)
9	0.26	<1	1,1,1-Trichloroethane	97(100)99(70)61(51)119(18)117(16)
10	0.34	10-100	Dichloropropane	63(100)62(70)41(50)39(35)65(30)76(26)
11	0.36	<1	Trichloroethylene	95(100)130(80)132(80)97(70)
12	0.45	<1	Tetramethylcyclopropane (T)	55(100)83(78)41(62)39,56(42)69(32)98(32)
13	0.49	<1	C_8H_{16}, e.g., Dimethylcyclohexane	55(100)97(67)69(45)112(20)
14	0.67	1-10	Tetrachloroethene	166(100)131(95)129(94)164(80)
15	1.00	-(8)	IS	75(100)77(33)

TABLE A-139. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 51E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	SI x 10^3
1	849	**	Chlorobenzene	112(100)77(76)114(32)51(29)50(28)74(12)	Benzene, chloro	598
2	999	*	Chlorocyclohexanol	57(100)80(26)81(18)98(8)105(3)134(2)116(1)	Cyclohexanol,4-chloro	564
3	1051	***	Nitrobenzene	77(100)51(70)123(36)50(29)65(16)93(14)	Benzene, nitro-	711
4	1073	*	Bromocyclohexanol	81(100)57(66)99(27)134(3)132(2)	Cyclohexanol,2-bromo	472
5	1100	*	Bromochlorocyclohexane	81(100)79(18)53(13)41(12)117(6)119(2)	Cyclohexane,1-bromo-2-chloro	451
6	1131	**	Nitrocyclohexene	81(100)79(86)53(69)41(51)97(21)127(4)		
7	1183	*	Halo-cyclohexane	81(100)89(29)41(28)57(26)55(25)79(23)127(5)128(3)		
8	1197	*	Halo-cyclohexane	81(100)41(33)55(29)57(26)79(23)98(7)		
9	1350	**	1,1'-Biphenyl	154(100)153(41)152(29)155(12)76(20)51(16)115(7)	1,1'-Biphenyl	581

TABLE A-140. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 52VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1		--	Air	44(100)
2	.15	10-100	Acetone	43(100)58(30)
3	.16	~100	Dichloromethane	49(100)84(35)
4	.18	1-10	Diisopropyl ether	45(100)43(65)41(15)87(10)59(8)69(2)
5	.22	10-100	Diisopropyl ether	43(100)45(90)41(48)87(40)59(30)69(10)
6	.25	1-10	1,1,1-Trichloroethane	97(100)61(78)
7	.33	1-10	Benzene	78(100)
8	.36	1-10	Bromodichloromethane	83(100)85(67)47(30)127(6)
9	.36	1-10	Trichloroethylene	95(100)60,97(73)62(50)132(31)
10	.41	1-10	C_8H_{16}: e.g. Trimethyl pentene	57(100)41(60)55(29) 39(19)69,97(5)112(4)
11	.52	>>100	Toluene	91(100)92(60)
	.57	>>100	Toluene	91(100)92(60)
	.61	>>100	Toluene	91(100)92(60)
12	.81	10-100	Chlorobenzene	112(100)77(80)
13	.90	~100	C_2 Alkyl benzene	91(100)106(30)
14	.92	10-100	C_2 Alkyl benzene	91(100)106(42)
15	.96	1-10	Cyclooctatetraene	104(100)78(55)103(50)51(40)77(28)
16	.98	1-10	C_2 Alkyl benzene	91(100)106(40)
17	1.00	~(8)	I.S.	75(100)77(13)
18	1.07	<1	C_3 Alkyl benzene	105(100)120(28)
19	1.12	<1	Chlorotoluene	91(100)126(20)89(18)128(9)
20	1.20	<1	Alkane	57(100)43(38)56(37)43(36)71(18)
21	1.23	<1	Dichlorobenzene	146(100)75(88)57,111(74)55(70)148(62)74(60)56(55)73,37(32)113(28)150(1
22	1.26	1-10	Dichlorobenzene	146(100)75(86)111(70)148(65)
23	1.29	1-10	Dichlorobenzene	146(100)148(62)111(57)75(52)
24	1.30	<1	C_4 Alkyl benzene	119(100) Sm 134
25	1.57	<1	Unknown	74(100)180(85)182(78)109(60)147(32)184(25)

TABLE A-141. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 52E

GC Peak No	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	SI x 10³
1	896	**	Methoxybenzene	108(100)78(79)65(74)93(18)51(16)109(8)	Benzene, Methoxy-	541
2	986	*	Chlorophenol	128(100)64(35)130(32)92(16)100(8)	Phenol, 2-Chloro-	455
3	1002	****	Phenol	94(100)66(85)65(56)40(64)95(12)	Phenol	470
4	1044	**	Bromophenol - #6	108(100)107(87)77(46)79(63)90(24)172(20)174(19)		
5	1047	**	Benzoic Acid - #6	105(100)77(60)136(36)51(20)	Benzoic Acid, Methyl Ester	415
6	1068	**	Methylphenol	107(100)108(82)77(34)79(24)109(6)	Phenol, 2-Methyl-	666
7	1091	**	Chlorophenol (methylated)	142(100)99(86)107(76)127(55)108(52)77(42)144(32)63(27)	Benzene, 1-Chloro-4-Methoxy	550
8	1135	**	Dimethylphenol	107(100)122(81)121(69)91(40)77(34)150(4)	Phenol, 2,4-Dimethyl	593
9	1169	**	Bromomethoxybenzene	186(100)187(97)143(59)145(58)63(42)92(30)171(41)173(40)	Benzene, 1-Bromo-2-Methoxy	412
10	1178	**	Methylbenzoic Acid	119(100)91(58)150(37)107(26)65(20)186(2)188(2)	Benzoic Acid, 3-Methyl-Methyl Ester	321
11	1285	**	Trichlorophenol (methylated)	195(100)197(97)167(61)169(59)210(56)212(51)214(17)97(20)	Benzene, 1,2,4-Trichloro-5-Methoxy	583
12	1626	**	Benzenesulfonamide N,4-Dimethyl	91(100)85(28)155(24)121(21)185(23)	Benzene Sulfonamide, N,4-Dimethyl	591
13	1818	**	Phenol, 2,6-[4(hydroxyphenyl)dimethyl]	108(100)52(18)77(12)91(11)214(36)181(24)183(7)		
14	1964	**	Phenol, 2-[4(Hydroxyphenyl)methyl]-	107(100)94(36)77(20)152(18)200(56)181(15)165(4)	Phenol, 2-[(4-Hydroxyphenyl) Methyl]	596
15	1978	**	C $\geq$ 18 Fatty Acid	74(100)87(84)143(26)199(9)255(4)298(3)	Heptadecanoic Acid, 16-Methyl, Methyl	583
					Ester	
16	2035	**	Phenol 2-[4-(Hydroxyphenyl)methyl]	107(100)77(28)152(18)153(16)200(85)199(41)201(11)	Phenol, 2[(4-Hydroxyphenyl) Methyl]	522
17	2302	**	1-Phenanthrenecarboxylic Acid Octahydro,	239(100)260(19)197(15)141(20)129(17)150(16)299(11)314(5)	1-Phenanthrenecarboxylic Acid Octahydro,	696
			1,4-Dimethyl-7-(1-Methylethyl) Methyl		1,4-Dimethyl-7-(1_Methylethyl) Methyl	
			Ester		Ester	

TABLE A-142. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 52E

GC Peak No	Retention Index	Amount, μg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	ΣI x 10^3
1	866	***	Cyclohexylamine	56(100)43(26)99(20)70(11)	Cyclohexan amine	595
2	890	***	Hydroxymethylimidazole #1	56(100)98(66)81(42)62(32)53(32)69(31)97(35)99(20)		
3	971	***	Ethanol, 2-(Diethylamino)	86(100)58(60)42(17)102(13)117(7)	Ethanol, 2-Diethylamino-	561
4	1032	**	Methylpyridine	93(100)66(32)65(16)92(12)94(6)	Pyridine, 3-Methyl	512
5	1381	**	5-Hexen-3yn-2one, 6-(1-Piperidinyl)	94(100)168(77)134(65)177(50)122(38)52(32)81(27)	5-Hexen-3-Yn-one,6(1-piperidinyl)	402
6	2017	*	1,2-Dicyclohexylurea	56(100)55(63)99(42)143(41)98(26)224(16)		

TABLE A-143. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 53VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.13	--	Air	44(100)
2	0.13	~1	Butene	41(100)56(70)39(41)
3	0.15	10-100	Acetone	43(100)58(25)
4	0.16	1-10	Dichloroethylene	61(100)96(90)98(55)63(33)
5	0.17	10-100	Dichloromethane	49(100)84(45)
6	0.18	10-100	Carbon disulfide	76(100)78(6)
7	0.21	1-10	Dichloroethylene	61(100)96(40)63(30)98(25)
8	0.22	10-100	Chloroform	83(100)85(60)47(55)
9	0.26	1-10	Trichloroethylene	97(100)61(90)99(60)117(6)
10	0.26	1-10	Methylbutyl adehyde (T)	44(100)41(76)43(62)58(52)71(20)86(3)
11	0.28	1-10	Benzene	78(100)
12	0.32	1-10	C_7H_{16}	43(100)41(50)56(49)57(40)85(18)71(15)100(2)
13	0.35	1-10	Bromodichloromethane	83(100)85(65) Small 127,129,131
14	0.35	1-10	Trichloroethylene	95(100)97(70)60(65)130(40)132(40)
15	0.53	10-100	Toluene	91(100)92(55)
16	0.56	10-100	Tetramethyltetrahydrofuran (T)	43(100)55(35)70(30)113(21)59(15)95(10)
17	0.68	1-10	Tetrachloroethene	166(100)131(96)129(80)164(78)94(65)96,168(40)
18	0.88	<1	C_2 Alkylbenzene	91(100)106(30)
19	0.90	1-10	C_2 Alkylbenzene	91(100)106(40)
20	0.98	1-10	C_2 Alkylbenzene	91(100)106(40)
21	1.00	-(8)	IS	75(100)
22	1.07	<1	C_9H_{20}	43(100)57(70)85(15)71(14) Sm 128

TABLE A-144. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 53E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10^3
1	886	***	Phenol	94(100)66(44)65(27)55(6)95(6)	Phenol	529
2	944	**	Chlorophenol + Methylphenol	108(100)107(96)77(48)79(43)51(18)90(22)142(6)144(2)	Phenol, 2-Methyl-	522
3	958	**	Benzoic Acid + Bromophenol	105(100)77(64)136(36)51(24)172(14)174(14)	Benzoic Acid, Methyl Ester	247
4	988	**	Methylphenol	107(100)108(83)77(36)79(25)51(12)53(10)	Phenol, 2-Methyl-	645
5	997	**	Chloromethylphenol + #4	107(100)108(56)77(41)142(27)144(8)	Phenol, 4-Chloro-2-Methyl-	350
6	1049	**	C ≥ 7 Fatty Acid	74(100)87(46)55(24)59(18)115(8)	Hexanoic Acid, 5-Methyl-, Methyl Ester	359
7	1099	**	Benzeneacetic Acid	91(100)150(27)65(18)89(8)59(6)	Benzeneacetic Acid, Methyl Ester	652
8	1110	**	Methylbromophenol + ?	107(100)77(60)120(54)92(43)152(26)186(60)188(59)		
9	1215	**	Benzenepropanoic Acid	104(100)91(56)105(37)164(28)77(22)128(16)65(14)51(10)133(8)	Benzene Propanoic Acid, Methyl Ester	507
10	1288	**	Trichlorophenol + Fatty Acid	74(100)87(62)143(20)55(20)59(14)	Decanoic Acid, Methyl Ester	260
11	1354	**	Methylbromophenol	107(100)186(84)188(84)77(76)51(24)121(10)151(8)		
12	1504	**	Dodecanoic Acid	74(100)87(71)55(20)43(17)143(14)214(2)	Dodecanoic Acid, Methyl Ester	653
13	1707	**	Tetradecanoic Acid	74(100)87(76)55(22)43(20)143(20)199(10)242(1)	Tetradecanoic Acid, Methyl Ester	607
14	1808	**	Pentadecanoic Acid	74(100)87(82)43(18)55(24)143(21)210(10)256(2)	Tetradecanoic Acid, 12-Methyl-Methyl Ester	422
15	1883	**	C ≥ 15 Fatty Acid	55(100)74(70)87(51)236(3)237(2)	10-Undecenoic Acid, Methyl Ester	408
16	1913	***	Hexadecanoic Acid	74(100)87(82)43(24)55(22)143(20)270(2)239(1)	Hexadecanoic Acid, Methyl Ester	689
17	2010	**	C ≥ 17 Fatty Acid	74(150)87(82)143(23)43(31)55(24)241(4)284(2)	Hexandecanoic Acid, 14-Methyl-, Methyl	508
					Ester	
18	2070	**	Octadecadienoic Acid	67(100)81(90)55(59)95(60)109(30)294(2)262(2)263(1)	9,11-Octadecadienoic Acid, Methyl Ester	528
19	2083	***	Octadecanoic Acid	55(100)69(74)74(72)87(57)97(56)264(7)265(5)296(1)	9-Octadecenoic Acid, Methyl Ester	742
20	2116	***	C ≥ 18 Fatty Acid	74(100)67(82)143(24)199(8)255(4)298(3)267(1)269(0.5)	Heptadecanoic Acid, 16-Methyl-, Methyl	702
					Ester	
21	2330	**	C ≥ 18 Fatty Acid	169(100)87(83)55(68)74(58)129(28)143(25)172(16)201(10)		
22	2415	*	C ≥ 18 Fatty Acid	74(100)87(90)143(30)283(4)326(4)	Hexadecanoic Acid, Methyl Ester	508
23	2518	*	C ≥ 19 Fatty Acid	74(100)87(84)143(28)	Triacontanoic Acid, Methyl Ester	507

TABLE A-145. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 53E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10^3
1	865	***	N,N-Dimethylacetamide	87(100)44(86)43(55)42(42)72(40)88(6)	N,N-Dimethylacetamide	623
2	1205	**	Quinoline	129(100)102(30)128(21)130(10)74(12)76(12)50(9)	Quinoline	739

TABLE A-146. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 54VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.12	--	Air	44(100)
2	0.15	10-100	Acetone	43(100)58(33)
3	0.16	10-100	Dichloroethylene	61(100)96(60)63(33)98(32)
4	0.16	>100	Need better spectrum	51(100)35(82)47(68)49(32)37(25)55(10)70(5)
5	0.19	<1	1,2-Dichloroethane	63(100)62(78)65(30)55(20)
6	0.19	1-10	2-Methylpentane	43(100)42(50)41(32)71(20)39(12)
7	0.20	1-10	3-Methylpentane	57(100)56(80)41(65)43(64)72(9)71(5)86(3)
8	0.21	1-10	Dichloroethylene	61(100)96(52)63(33)98(30)
9	0.22	>10	Chloroform	83(100)85(67)
10	0.24	<1	Tetrahydrofuran + C_6H_{12}	41(100)69(57)42(50)39,84(23)
11	0.25	1-10	Methyl cyclopentane	56(100)41(65)69(30)55(22)84(4)
12	0.26	10-100	1,1,1-Trichloroethane	97(100)99(66)117(12)119(10)
13	0.28	10-100	Benzene	78(100)
14	0.30	<1	Cyclohexane	56(100)41(65)84(48)55(32)69(25)
15	0.33	<1	Alkane	43(100)41(55)56(50)57(60)42(32)71(15)85(8)
16	0.34	<1	C_7H_{16} Alkane	43(100)41,57(46)71(41)56,70(32)85(5)100(2)
17	0.36	10-100	Trichloroethylene	95(100)97(67)130(60)132(58)
18	0.41	<1	C_7H_{16} Alkane	43(100)41(60)57(40)71(35)100(10)
19	0.46	1-10	C_7H_{14} Alkene	55 (100)83(80)41(61)42(38)98(30)
20	0.55	10-100	Toluene	91(100)92(60)
21	0.68	1	C_8H_{16}	55(100)41(55)97(50)56(32)42(28)69(21)83(11)112(10)
22	0.69	1-10	1,1,2,2 Tetrachloroethene	129(100)166(95)131(90)164(78)96(75)
23	0.70	<1	C_8H_{16}	55(100)57(60)41(65)112(15)
24	0.71	1-10	C_8H_{18} Alkane	43(100)57(30)85(20)71(15) Sm 114
25	0.80	1	Chlorobenzene	112(100)77(95)51(60)
26	0.82	1-10	C_8H_{16}	55(100)83(75)41(62)82(38)112(10)
27	0.87	1	Alkane	57(100)43(68)41(40)97,99(10)
28	0.88	10-100	C_2 Alkyl benzene	91(100)106(30)
29	0.89	1	C_9H_{18}	69(100)55(90)111(60)41(55)56(40)126(12)
30	0.91	10-100	C_2 Alkyl benzene	91(100)106(50)

TABLE A-146. (Continued)

GC Peak No	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
31	.91	1	Hydrocarbon	43(100)86,41(72)85(18)57(17)
32	.96	<1	C_9H_{18}	43(100)57(25)85(15)111(8)126(5)
33	.97	<1	C_2 Alkyl benzene T	55(100)91(60)106(30)
34	.98	10-100	C_2 Alkyl benzene	91(100)106(45)
35	1.00	-(8)	IS	75(100)
36	1.00	1-10	C_9H_{18} Alkene	55(100)97(40)41(38)69(18)126(3)
37	1.05	1-10	C_9H_{18} Alkene	55(100)97(62)41(40)69(30)126(10)
38	1.07	1-10	C_9H_{20} Alkene	43(100)57(68)85(17)71(11)128(1)
39	1.08	1-10	C_3 Alkyl benzene	105(100)120(25)
40	1.12	1-10	Alkyl benzene	55(100)83(85)82,41(45)126(5)
41	1.16	10-100	C_3 Alkyl benzene	91(100) 120(12)
42	1.16	1-10	Alkane	57(100)43(70)71(55)41(50)56(30)113(8)
43	1.18	10-100	C_3 Alkyl benzene	105(100)120(32)
44	1.18	10-100	C_3 Alkyl benzene	105(100)120(90)
45	1.20	10-100	C_3 Alkyl benzene	105(100)120(50)
46	1.22	10-100	C_3 Alkyl benzene	105(100)120(30)
47	1.24	1-10	$C_{10}H_{20}$, eg. C_4 Alkylcyclohexane	55(100)97(50)96(30)81(15)140(3)
48	1.25	10-100	C_3 Alkyl benzene	105(100)120(60)
49	1.27	<10	Dichloro benzene	146(100)148(65)111(58)113(18)150(10)
50	1.29	1-10	C_4 Alkyl benzene	91(100)134(20)
51	1.29	1-10	C_4 Alkyl benzene	105(100)134(20)
52	1.32	10-100	Dichlorobenzene + Alkane	43(100)57(90)41(62)71(32)146(25)148(7)
53	1.33	1-10	C_4 Alkyl benzene	119(100)91(12)134(22)
54	1.33	<10	Methyl Styrene	117(100)118(55)115(32)91(22)119(16)
55	1.35	<10	$C_{10}H_{16}$ e.g. Limonene	68(100)67(77)93(60)107(11)121(10)136(5)
56	1.37	<10	Hydrocarbon	43(100)57(70)71(70)85(50)
57	1.38	<10	C_4 Alkyl benzene	105(100)119(90)134(60)
58	1.38	10-100	C_4 Alkyl benzene	105(100)134(20)

TABLE A-147. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 54E

GC Peak No.	Retention Index	Amount, µg^a	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	KI x 10^3
1	858	**	Xylene	91(100)106(62)		
2	863	**	C_3-Alkylbenzene	105(100)120(67)77(11)		
3	869	**	C_3-Alkylbenzene	105(100)120(28)57(38)		
4	876	**	C_3-Alkylbenzene	105(100)40(99)41(90)120(44)77(20)91(17)121(6)		
5	899	**	C = 10 alkane	11(100)40(96)57(58)71(28)85(18)142(2)		
6	901	**	C_3-Alkylbenzene	105(100)120(36)77(16)91(15)51(8)65(6)		
7	957	**	C_4-Alkylbenzene	119(100)134(26)91(23)		
8	973	**	C_4-Alkylbenzene	119(100)134(22)		
9	981	**	C = 11 alkane	62(100)43(96)41(96)57(96)71(97)85(56)156(5)157(0.5)	Decane,4-methyl	411
10	1005	**	C_4-Alkylbenzene	119(100)40(89)134(35)91(26)	Benzene,1-methyl-4-(1-methyl ethyl)	373
11	1089	**	C_5-Alkylbenzene	133(100)119(61)91(33)148(33)		
12	1103	***	Dodecane	57(100)42(98)43(97)41(86)58(88)71(92)85(90)170(6)		
13	1206	***	Tridecane	62(100)41(89)43(67)57(84)71(70)98(16)85(16)184(0.3)	Tridecane,4,8-dimethyl	660
14	1268	***	Methylnaphthalene	142(100)141(97)41(82)115(60)143(13)160(2)	Naphthalene,1-methyl	276
15	1283	**	Methylnaphthalene	142(100)141(99.5)41(92)115(69)143(14)		
16	1304	***	Tridecane	43(100)57(94)71(96)85(91)99(18)184(4)185(0.2)	Tridecane	378
17	1367	**	C > 13 Alkane	43(100)57(63)141(63)71(31)85(20)115(18)156(24)193(3)		
18	1381	***	C > 13 Alkane	43(100)57(86)71(88)85(48)113(12)127(12)183(1)		
19	1393	**	Dimethylnaphthalene	156(100)141(87)115(27)128(20)155(35)157(12)	Naphthalene,1,2-dimethyl	462
20	1403	***	Dimethylnaphthalene + Tetradecane	58(100)44(99.5)85(94)71(90)141(76)156(77)198(4)		
21	1468	***	C > 14 Alkane + ?	85(96)71(88)57(82)58(79)55(66)99(33)141(11)183(3)		
22	1505	***	Pentadecane	71(100)58(99)44(99)85(90)99(34)155(20)212(1)		
23	1524	**	C ≥ 15 Alkane	43(100)57(58)55(56)83(68)97(16)169(7)		
24	1550	**	C > 15 Alkane + ?	43(100)57(50)71(48)85(30)		
25	1604	***	Hexadecane	71(100)58(99)44(98)85(84)99(43)113(24)169(11)227(1)	Hexadecane	306
26	1655	***	C > 16 Alkane	58(100)42(91)85(82)71(74)99(30)113(26)169(10)		
27	1705	***	Heptadecane	71(100)58(99)44(99)85(88)99(42)113(24)127(14)240(1)		
28	1715	***	C 17 Alkane	71(100)58(98)44(81)85(80)99(35)113(42)127(16)		
29	1805	***	Octadecane	71(100)58(99)44(98)85(88)99(46)113(28)		
30	1817	**	C 18 Alkane	43(100)71(86)57(76)85(75)113(23)127(18)	Hexadecane,2,6,10,14-tetramethyl	500

TABLE A-147. (Continued)

GC Peak No	Retention Index	Amount, μg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10³
31	1906	**	Nonadecane	43(100)58(98)85(90)71(84)99(37)113(22)127(13)		
32	2003	**	Eicosane	43(100)85(96)71(96)57(90)99(31)113(19)127(12)	Eicosane,10-methyl	510
33	2106	**	Heneicosane	41(100)57(96)71(64)85(42)99(12)113(6)		

TABLE A-148. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 54E

GC Peak No.	Retention Index	Amount, μg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10³
1	952	***	Methylpyridine	93(100)66(33)65(17)92(12)94(7)	Pyridine, 3-Methyl-	507
2	1034	**	Methylaniline	106(100)107(80)77(30)79(25)51(16)65(13)	Benzenamine, N-Methyl	687
3	1061	**	Dimethylaniline	120(100)127(72)77(30)104(18)105(16)51(12)122(6)	1,2-Ethanediamine, N,N'-Dimethyl-N,N-	601
					diphenyl	
4	1100	*	C_3-Alkylpyridine	106(100)121(34)77(24)65(12)51(11)127(5)134(2)	Benzenamine, N-Ethyl-	530
5	1135	**	Dimethylaniline	121(100)106(98)120(96)77(23)91(18)65(9)51(10)	Pyridine, 3 Ethyl-5-Methyl	427
6	1167	**	Chlorotoluene	121(100)129(32)65(26)92(19)100(16)	Benzenamine, 4-Chloro	625
7	1200	*	N,N-Diethylaniline	134(100)106(50)77(34)149(27)51(10)		
8	1255	**	Acetamide, N-(4-Bromophenyl)	171(100)173(100)65(51)92(45)142(20)141(17)		
9	1316	*	Pyridine 3(-1-Methyl-2-Pyrrolidinyl)	84(100)133(68)161(26)162(21)	Pyridine,3-(1-Methyl-2-Pyrrolidinyl)	632

TABLE A-149. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 55VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.13	--	Air	44(100)
2	.15	500-1000	Acetone	43(100)58(40)
3	.16	1-10	Unknown (weak)	45(100)43(63)46(37)41(12)53(5)55(4)
4	.17	500-1000	Dichloromethane	49(100)84(40)
5	.23	~20	Chloroform	83(100)85(67)
6	.24	~10	Diisopropyl ether	45(100)43(40)87(18)59(12)69(4)
7	.26	<1	Tetrahydrofuran	42(100)71(30)41,72(30)85(10) ?
8	.27	<1	1,1,1-Trichloroethane	97(100)61(80)99(67)
9	.30	~1	Benzene	78(100)
10	.35	1-10	Cyclohexene	67(100)54(78)39(46)41,82(38)
11	.37	1-10	Bromodichloromethane	83(100)85(60)47(28)129(8)
12	.46	1-10	C_8H_{16}, e.g. Trimethyl pentene	57(100)41(50)55(30)69,97,112(6)
13	.57	>>100	Toluene	91(100)92(60)
14	.61	<1	Dibromochloromethane	129(100)127(80)131(40)
15	.89	1-10	Ethyl benzene	91(100)106(30)
16	.92	1-10	m-,p-xylene	91(100)106(42)
17	.98	1-10	o-Xylene	91(100)106(40)
18	1.00	-(8)	I.S.	75(100)77(33)
19	1.26	10-20	Dichlorobenzene	146(100)148(68)75,111(56)
20	1.31	10-20	Dichlorobenzene	146(100)148(62)75,111(63)

TABLE A-150. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 56VE

GC Peak No	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.11	--	Air	44(100)
2	.14	~10	Trichlorofluoromethane	101(100)103(67)
3	.16	10-100	Dichloromethane	49(100)84(60)
4	.22	~100	Diisopropyl ether	43(100)45(100)41,87(44)59(28)
5	.29	10-100	Benzene	78(100)
6	.35	1-10	Bromodichloromethane	83(100)85(67)129(6)127(4)
7	.54	10-100	Toluene	91(100)92(60)
8	.79	10-100	Chlorobenzene	112(100)77(90)114(33)
9	.88	1-10	C_2 Alkyl benzene	91(100)106(30)
10	.91	1-10	C_2 Alkyl benzene	91(100)106(45)
11	.98	1-10	O-xylene	91(100)106(42)
12	1.00	-(8)	I.S.	75(100)77(33)
13	1.25	10-100	Dichlorobenzene	146(100)148(67)
14	1.29	~10	Dichlorobenzene	146(100)148(67)

TABLE A-151. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 56E

GC Peak No	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	SI $\times 10^3$
1	861	*	Chlorobenzene	112(100)77(68)114(34)50(28)51(25)	Benzene,chloro	571
2	867	*	Xylene	91(100)59(42)106(29)57(14)		
3	873	**	Xylene	91(100)106(44)105(23)77(14)	Benzene,1,2-dimethyl	563
4	899	***	$CH_3CH_2-O(CH_2O)_x-C_2H_5$ polymer	76(100)74(50)41(35)105(20)135(2)		
5	921	**	Homolog of #4	45(100)75(70)105(20)135(7)		
6	987	*	Dichlorobenzene	146(100)148(64)111(51)75(48)113(18)150(11)	Benzene,1,4-dichloro	561
7	1008	*	Dichlorobenzene	146(100)148(63)111(52)75(48)30(28)150(11)	Benzene,1,2-dichloro	502
8	1035	*	Dichlorobenzene	146(100)111(50)148(44)67(37)		
9	1078	***	Homolog of #4	105(96)91(28)135(14)107(16)		
10	1108	***	?	61(100)41(85)91(34)43(30)121(2)		
11	1122	**	?	78(100)106(43)136(28)51(20)137(2)		
12	1149	*	Trichlorobenzene	180(100)182(97)74(46)109(40)145(39)184(30)147(26)	Benzene,1,2,4-trichloro	447
13	1181	*	Trichlorobenzene	180(100)	Benzene,1,2,4-trichloro	450
14	1256	***	Homolog of #4	45(100)75(78)105(38)107(12)135(10)		
15	1297	**	?	112(100)77(95)140(65)51(43)114(32)142(24)170(24)172(12)		
16	1431	***	Homolog of #4	45(100)75(75)105(45)107(20)135(20)165(2)		
17	1591	**	Homolog of #4	45(100)25(70)105(56)135(33)107(22)165(5)		
18	1605	***	Homolog of #4	135(100)105(100)107(89)91(55)121(37)165(13)		
19	1774	**	Homolog of #4	45(100)75(80)105(70)135(45)165(12)195(2)		
20	1955	**	Homolog of #4	45(100)75(70)105(60)135(44)165(24)195(3)		

TABLE A-152. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 56E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	SI x 10^3
1	909	***	? Mixture	61(100)91(34)60(24)44(18)89(14)121(1)		
2	989	*	Chlorophenol	128(100)130(32)64(35)63(29)92(16)	Phenol, 2-Chloro-	493
3	1017	****	Phenol	94(100)66(50)65(30)40(26)95(6)	Phenol	473
4	1058	**	Polymer ?	65(100)75(84)105(28)135(6)107(6)		
5	1070	**	Chlorobenzoic Acid	105(100)77(70)136(33)51(26)172(6)174(6)	Benzoic Acid, Methyl Ester	453
6	1101	**	Mixture	61(100)91(22)44(11)107(10)108(8)121(1)119(0.5)		
7	1143	*	Dichlorophenol + ?	120(100)92(77)152(49)63(28)161(32)176(30)178(18)		
8	1169	**	Homolog of #4	65(100)75(64)105(35)135(11)117(10)136(1)		
9	1241	**	Homolog of #4	65(100)75(69)105(48)135(22)107(18)165(1)		
10	1818	**	Phenol, 2,6-[4-(Hydroxyphenyl)dimethyl]	108(100)214(<1)181(26)152(20)77(15)215(6)		
11	1967	**	Phenol, 2-[4-Hydroxyphenyl)methyl]-	107(100)200(70)94(37)77(27)152(23)181(20)201(10)	Phenol, 4,4'-Methylenebis-	490
12	2009	**	Heptadecanoic Acid + ?	55(100)74(69)87(54)200(24)264(6)		
13	2040	**	C ≥ 17 Fatty Acid	74(100)87(83)143(24)199(10)255(4)298(2)	Heptadecanoic Acid, 16-Methyl-, Methyl Ester	568

TABLE A-153. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 56E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	SI x 10^3
1	882	***	Mixture ?	82(100)55(68)68(47)83(42)96(11)110(4)	Hexanedinitrile, 2-Methyl	402
2	916	****	Mixture ? MW 121	61(100)91(55)41(28)89(20)121(4)		
3	991	**	Isomer of #2	61(100)91(27)44(13)60(10)121(2)		
4	1059	**	Hexamethylenetetramine	42(100)140(75)85(22)112(12)141(6)		
5	1100	**	Hexamethylenetetramine	42(100)140(75)85(22)112(12)		
6	1291	**	Homolog #2	61(100)91(34)89(31)119(4)121(6)149(1)		

TABLE A-154. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 57VE

GC Peak No	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.12	--	Air	44(100)
2	.13	1-10	Unknown	60(100)44(5)45(3)
3	.16	~100	Trimethyl Silonol	75(100)45(99)
4	.22	~30	Chloroform	83(100)85(67)
5	.22	~10	Diisoporpyl ether	45(100)43(42)87(15)59(12)
6	.29	>>100	Benzene	78(100)
7	.53	1-10	Toluene	91(100)92(55)
8	.80	~100	Chlorobenzene	112(100)77(85)114(35)
9	1.00	-(8)	I.S.	75(100)77(33)
10	1.14	~80	Chlorotoluene	91(100)126(28)128(10)
11	1.15	1-10	Chlorotoluene	91(100)126(21)128(7)
12	1.26	20-30	Dichlorobenzene	146(100)75(77)111(67)148(65)
13	1.27	100-200	Dichlorobenzene	146(100)148(67)111(55)75(52)
14	1.30	80-100	Dichlorobenzene	146(100)148(67)111(40)75(52)

TABLE A-155. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 57E

GC Peak No	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	KI x 10^3
1	902	***	Methylphenol	108(100)78(84)65(80)93(20)51(18)109(10)	Benzene, Methoxy-	556
2	1007	****	Chlorophenol + Phenol	66(100)94(99)65(92)55(24)50(19)128(8)130(2)	Phenol	452
3	1074	**	Benzoic Acid	105(100)77(98)136(78)51(46)50(21)	Benzoic Acid, Methyl Ester	541
4	1095	**	Chloromethylphenol	142(100)99(88)127(56)144(32)101(29)129(19)	Benzene, 1-Chloro-4-Methoxy	626
5	1172	**	Bromomethylphenol	186(100)188(96)143(65)145(63)171(41)173(40)63(34)77(18)	Benzene, 1-Bromo-2-Methoxy	637
6	1212	**	Phenoxyethanol	94(100)138(30)77(30)66(20)56(11)139(2)	Ethanol, 2-Phenoxy-	625

TABLE A-156. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 58VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.12	--	Air	44(100)
2	.13	~10	Propene (T)	41(100)39(80)42(70)40(28)
3	.16	100-200	Acetone	43(100)58(100) (Sat'd)
4	.17	100-200	Isopropyl alcohol	45(100)41(22)43(20)
5	.23	1-10	Chloroform	83(100)85(65)
6	.27	~1	1,1,1-Trichloroethane	97(100)61(75)99(65)117,119(12)
7	.53	1-10	Unknown	59(100)43(77)77(22)103(15)
8	.55	1-10 ea	Toluene + Unknown	39(100)63(75)91(40)41(33)65(27)92(23)
9	.56	<1	Chloropropene	76(100)41(35)78(30)
10	1.00	-(13)	I.S.	75(100)77(33)

TABLE A-157. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 58E

GC Peak No	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10^3
1	1116	**		78(100)106(70)136(51)51(40)		
2	1284	**	Benzenemethanol, methoxy-acetate	120(100)91(93)92(78)77(20)180(18)149(13)65(13)	Benzenemethanol,AR-methoxy-acetate	404
3	1452	**	Mixture + Alkylbenzene	91(98)147(96)119(94)55(78)57(76)162(46)192(24)		
4	1660	**	Chloro-hydrocarbon	41(100)55(32)57(32)91(25)69(19)71(18)105(8)		
5	1780	**	?	177(100)91(35)108(33)77(26)57(21)192(11)222(11)		
6	1978	**	?	134(100)57(72)79(68)107(66)167(25)166(25)234(6)		
7	2025	**	Isomer of ? 9	79(100)137(100)138(96)107(81)119(54)179(15)193(8)		
8	2031	**	Chloro-hydrocarbon	41(100)79(33)137(26)138(26)107(26)43(20)69(17)193(1)		
9	2039	**	?	83(100)55(49)134(36)79(31)166(18)232(4)204(2)205(1)233(1)		
10	2121	**	?	156(100)58(98)212(25)84(17)98(8)213(4)		
11	2320	**	C ≥ 24 Alkane	41(100)57(34)71(22)85(16)99(5)	Heptadecane,9-octyl	619
12	2713	**	?	58(100)84(16)212(29)240(7)241(5)		
13	2913	**	?	58(100)43(45)64(14)70(8)268(38)212(43)		

TABLE A-158. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 58E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	R.I. x 10^3
1	902	***	Methoxybenzene	108(100)65(77)78(72)77(24)51(18)93(16)109(7)	Benzene Methoxy	551
2	990	***	Chlorophenol + Phenol	128(100)61(58)64(32)130(32)92(16)100(8)	Phenol, 2-Chloro-	324
3	1044	**	Methylphenol + Bromophenol	108(100)107(87)77(42)79(41)90(23)51(14)172(1)174(1)	Phenol, 2-Methyl-	629
4	1073	*	Benzoic Acid	105(100)77(74)136(32)51(28)	Benzoic Acid, Methyl Ester	333
5	1092	**	Methoxychlorobenzene	142(100)99(85)127(54)107(38)63(24)144(32)129(18)	Benzene, 1-Chloro-4-Methoxy-	586
6	1112	*	C $\geq$ 7 Fatty Acid	74(100)87(52)115(10)127(10)135(3)136(3)	Hexanoic Acid, 5-Methyl-, Methyl Ester	327
7	1170	**	Dimethylphenol + C_4-Phenol	107(100)122(86)121(52)91(37)77(33)150(4)	Benzene, 1-Methoxy-2-Methyl-	465
8	1189	**	Methylbromophenol + Dichloromethoxyl-	161(100)133(96)176(90)163(64)135(64)178(56)186(58)188(56)		
			benzene			
9	1220	*	Benzene, [(methoxymethoxy)methyl]	91(100)120(76)92(33)152(32)77(19)121(16)65(12)153(3)		
10	1232	*	C $\geq$ 9 Fatty Acid	74(100)87(60)163(11)		
11	1263	**	Dichlorophenol (Methylated)	161(100)176(87)133(84)163(63)178(58)222(19)220(14)224(5)	Benzene, Dichloromethoxy-	399
12	1273	*	Hydroxymethylbenzoic Acid	106(100)134(95)166(48)77(41)78(31)105(37)135(36)211(3)	Benzoic Acid, 2-Hydroxy-3-Methyl, Methyl	536
					Ester	
13	1282	*	C_4-Alkylphenol	135(100)107(43)150(16)95(12)91(10)77(9)131(10)	Phenol, 4-(1,1-Dimethyl Ethyl)-	683
14	1309	*	C $\geq$ 10 Fatty Acid + Trichlorophenol	Mixed Spectrum		
15	1338	*	Bromophenol + ?	172(100)174(98)107(70)65(53)77(43)150(39)93(23)		
16	1357	*	Chloroalkylphenol + ?	91(100)120(50)163(40)207(9)222(9)205(6)220(6)		
17	1436	*	Chlorobromo-Subst.-Phenol	241(100)256(83)239(67)213(59)164(57)243(50)255(53)258(40)		
18	1499	*	Dimethoxybenzaldehyde	166(100)165(60)95(44)151(15)167(10)	Benzaldehyde, 3,4-Dimethoxy	553
19	1794	*	Benzene, 1-Methoxy-2-[(Methoxyphenyl)	228(100)91(98)107(97)197(76)181(64)152(57)229(15)	Benzene, 1-Methoxy-2-[(4-Methoxyphenyl)	386
			methyl]		methyl]	
20	1825	***	?	108(100)214(70)181(43)107(36)152(35)153(25)215(10)		
21	1856	**	C $\geq$ 16 Fatty Acid	74(100)87(85)143(23)227(6)270(2)228(2)	Hexadecanoic Acid, Methyl Ester	483
22	1896	**	Homolog or Isomer of #20 ?	108(100)121(24)152(22)214(56)197(17)228(8)		
23	1974	***	?	214(100)108(84)183(63)121(53)77(32)213(45)215(14)		
24	2048	***	Phenol, 2-[(4-Hydroxyphenyl)methyl]-	200(100)94(99)107(97)77(54)152(40)181(37)199(26)201(18)	Phenol, 2-[(4-Hydroxyphenyl)Methyl]-	548
25	2113	*	C $\geq$ 18 Fatty Acid	74(100)87(88)143(20)298(2)		
26	2113	*	Isomer of #24	107(100)200(75)199(65)	Phenol, 2[(4-Hydroxyphenyl)Methyl]-	537

TABLE A-158. (Continued)

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10^3
27	2304	**	Octahydro C_5 Alkylphenanthrene	239(100)240(21)197(18)299(12)314(6)355(3)	1-Phenanthrene Carboxylic Acid, 1,2,3,4,	556
			Carboxylic Acid M.E.		4A,9,10,10A-Octahydro-1,4A-Dimethyl-7-	
					(1-Methyl Ethyl)-Methyl Ester	
28	2398	*	Isomer of #27	237(100)238(20)312(10)297(8)313(2)		
29	2784	**	?	121(100)107(18)91(26)227(25)228(13)334(22)335(6)		
30	2799	***	Isomer of #29	107(100)213(41)91(34)121(23)226(10)334(18)335(5)		

TABLE A-159. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 59VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.12	--	Air	44(100)
2	.15	10-100	Acetone	43(100)58(25)
3	.15	~1	Diethyl ether	45(100)59(98)74(51)
4	.16	1-10	Dichloromethane	49(100)84(37)
5	.19	1-10	Dichloroethane	63(100)65(30)83(15)98(6)100(4)
6	.22	~1	Chloroform	49(100)83(55)85(42)130(31)128(27)132(10)
7	.26	1-10	1,1,1-Trichloroethane	97(100)61(72)99(67)117,119(10)
8	.28	<1	Benzene	78(100)
9	.35	10-100	Trichloroethylene	95(100)132(70)128(68)97(61)
10	.45	<1	C_7H_{14} Alkene	55(100)83(80)41(60)42(40)69,98(25)
11	.54	10-100	Toluene	91(100)92(60)
12	.97	-(8)	I.S.	75(100)77(33)

TABLE A-160. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 60VI

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.12	--	Air	44(100)
2	.15	70-80	Furan	38(100)68(95)43(25)58(5)
3	.16	~100	Dichloromethane	49(100)84(85)51(67)
4	.18	1-10	Dichloroethylene	61(100)96(92)98(62)100(12)
5	.20	80-100	Dichloroethylene	61(100)96(88)98(52)63(44)
6	.23	80-100	Chloroform	83(100)85(90)47(52)
7	.24	200-300	Tetrahydrofuran	42(100)72(32)71(31)
8	.26	1-10	1,1,1-Trichoroethane	97(100)61(65)97(62)117,119(10)
9	.29	90-100	Benzene	78(100)
10	.37	100-130	Trichloroethylene	95(100)130(78)138(73)97(61)
11	.55	50-60	Toluene	91(100)92(60)
12	.58	1-10	Dibromochloromethane	129(100)127(80)79,81(29)
13	.68	50-70	Tetrachloroethene	166(100)129(93)131(88)164(80)94(58)47(48)
14	.80	60-80	Chlorobenzene	112(100)77(75)
15	.86	1-10	m-Chlorobenzotrifluoride	180(100)145(82)75(70)161(68)50(62)
16	.88	1-10	C_2 Alkyl benzene	91(100)106(30)
17	.91	10-20	C_2 Alkyl benzene	91(100)106(42)
18	.98	10-20	O-xylene	91(100)106(45)
19	.99	1-10	1,1,2,2-Tetrachloroethane	83(100)85(67)60,61,95(15)131,133(5)166,168(2)
20	1.00	-(8)	I.S.	75(100)77(33)
21	1.08	1-10	C_3 Alkyl benzene	105(100)120(26)
22	1.13	10-20	C_3 Alkyl benzene	91(100)120(30)
23	1.14	~10	C_3 Alkyl benzene + ?	91(100)121(28)63(16)120(12)123(11)
24	1.16	1-10	C_3 Alkyl benzene	91(100)120(20)
25	1.18	10-20	C_3 Alkyl benzene	105(100)120(30)
26	1.19	~10	C_3 Alkyl benzene	105(100)120(25)
27	1.20	1-10	C_3 Alkyl benzene	105(100)120(40)
28	1.22	1-10	C_3 Alkyl benzene	105(100)120(30)
29	1.26	10-20	C_3 Alkyl benzene	105(100)120(40) + small dichlorobenzene ~ 1 ppb
30	1.27	1-10	Dichlorobenzene	146(100)148(65)111(50)75(48)

TABLE A-161. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 60VE

GC Peak No	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	0.03	500-1000	Acetone	43(100)58(100) Sat'd
2	0.04	40-50	Dichloromethane	49(100)84(65)
3	0.09	1-10	Methyl ethyl ketone	43(100)72(18)57(5)
4	0.10	10-20	Dichloroethylene	61(100)96(60)98(38)
5	0.11	60-70	Chloroform	83(100)85(63)
6	0.13	10-20	Tetrahydrofuran	42(100)41(52)72(28)71(27)
7	0.15	1-10	1,1,1-Trichloroethane	97(100)99(66)61(55)117,119(12)
8	0.17	10-20	Benzene	78(100)
9	0.18	1-10	Carbon tetrachloride	117(100)119(95)47(47)82(37)
10	0.22	1-10	2-Pentanone	43(100)86(10)58(6)71(5)
11	0.25	30-40	Trichloroethylene	95(100)130(86)132(82)97(63)
12	0.29	<1	Benzotrifluoride	146(100)91(62)127(58)141(52)
13	0.47	90-100	Toluene	91(100)92(60)
14	0.62	70-80	1,1,2,2-Tetrachloroethene	166(100)129(90)131(87)164(78)
15	0.76	10-20	Chlorobenzene	112(100)77(72)114(33)
16	0.85	<1	Ethyl benzene	91(100)106(33)
17	0.89	1-10	m- + p-Xylene	91(100)106(67)
18	0.97	1-10	o-Xylene	91(100)106(45)
19	1.00	-(8)	I.S.	75(100)77(33)
20	1.09	~1	C_3 Alkyl benzene	105(100)120(25)
21	1.16	20-30	C_3 Alkyl benzene + ?	91(100)121(30)89(17)63(16)123(11)120(9)
22	1.18	1-10	C_2 Alkyl benzene + ?	91(100)121(24)63(15)65(10)89(9)120(9)123(8)
23	1.21	1-10	C_3 Alkyl benzene	105(100)120(25)
24	1.22	1-10	C_3 Alkyl benzene	105(100)120(22)
25	1.24	<1	C_3 Alkyl benzene	105(100)120(62)
26	1.26	~1	C_3 Alkyl benzene	105(100)120(25)
27	1.30	1-10	C_3 Alkyl benzene	105(100)120(40)
28	--	1-10	Dichlorobenzene	146(100)148(65)75(57)111(52)
29	--	1-10	Dichlorobenzene	146(100)75(95)111(88)50(71)148(60)

TABLE A-162. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 601

GC Peak No	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biomass Match	
					Compound	RI x 10³
1	834	*	Tetrachloroethene	129(100)131(95)166(92)164(75)168(44)170(10)	Benzene, tetrachloro	568
2	849	**	Chlorobenzene	112(100)113(98)114(77)77(97)51(97)		
3	854	**	?	57(99)83(98)69(81)86(77)97(25)180(5)182(1)		
4	873	*	Ethylbenzene	91(100)106(82)92(75)77(35)51(40)	Benzene,1,2-dimethyl	495
5	870	**	Ethylbenzene	92(100)91(95)106(86)105(39)51(40)77(37)55(25)65(24)	Benzene,1,2-dimethyl	439
6	883	**	Tetrachloroethane	83(100)86(98)131(22)133(20)168(11)166(9)170(5)		
7	888	*	Butoxyethanol	57(100)45(67)41(53)87(20)75(10)100(2)	Ethanol,2-butoxy	848
8	910	*	C_3- Alkylbenzene	105(100)77(25)51(23)120(19)	Benzene,1-methyl ethyl	712
9	930	**	Chloromethylbenzene	91(100)92(60)126(47)89(36)63(33)128(14)	Benzene(chloromethyl)	305
10	935	**	Chloromethylbenzene + C_3-Alkylbenzene	91(100)92(68)65(29)120(19)51(15)	Benzene(chloromethyl)	405
11	944	**	C_3- Alkylbenzene	105(100)120(58)77(43)79(35)91(30)51(25)65(20)	Benzene,1-ethyl-2-methyl	562
12	960	**	C_3-Alkylbenzene	105(100)120(25)57(27)77(16)74(14)91(14)	Benzene(1-methyl ethyl)	395
13	976	**	C_3-Alkylbenzene	105(100)120(72)106(66)77(37)91(27)79(26)51(26)121(7)	Benzene(1,2,4-trimethyl)	562
14	985	**	1,3-Dichlorobenzene	75(100)111(99)148(98)146(97)50(75)113(31)150(15)	Benzene(1,4-dichloro)	430
15	1000	**	Decane	57(100)71(49)85(26)99(5)98(4)142(2)	Decane	502
16	1007	**	1,4-Dichlorobenzene	148(100)146(95)111(98)75(98)50(65)113(21)150(16)	Benzene,1,4-dichloro	400
17	1022	**	Dichlorocyclohexane + C_3-Alkylbenzene	80(100)81(99)82(91)77(98)105(96)51(61)120(15)152(1)154(0.6)	Cyclohexane,1,3-dichloro	237
18	1068	**	C_4 Alkylbenzene + ?	58(100)82(97)81(83)99(76)132(7)134(7)180(1.6)178(1.5)		
19	1099	**	Undecane + ?	57(100)71(96)85(50)156(3)		
20	1110	**	Bromochlorocyclohexane	82(100)81(99)79(43)53(38)117(16)119(6)		
21	1126	**	C ≤ 11 Alkane	57(100)43(59)71(50)85(16)117(14)133(7)184(0.3)186(0.3)		
22	1146	**	1,2,4-Trichlorobenzene	180(100)74(71)109(52)145(45)147(28)111(17)182(92)184(29)	Benzene,1,2,3-trichloro	496
23	1151	**	Naphthalene	128(100)51(29)64(19)63(18)119(15)102(14)127(14)129(11)	Naphthalene	685
24	1178	**	C ≥ 11 Alkane	57(100)71(53)85(27)120(4)160(2)161(1.7)	Decane	648
25	1200	**	Dodecane + ?	58(100)71(97)85(56)98(8)99(7)170(0.7)	Dodecane	321
26	1228	**	C_3-Alkylbromobenzene	119(100)198(20)200(20)91(40)77(20)	Benzene,2-bromo-1,3,5-trimethyl	586
27	1453	**	?	57(100)55(31)165(19)137(12)180(8)179(3)		
28	1556	**	C ≥ 15 Alkane + ?	74(100)56(97)85(95)100(56)165(4)143(2)167(2)175(1)		
29	1989	**	C ≥ 19 Alkane + ?	60(100)73(98)57(86)55(80)129(25)256(0.5)		
30	2000	**	[illegible]	[illegible]		

TABLE A-162. (Continued)

GC Peak No.	Retention Index	Amount, µg?	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	SI x 10^3
31	2035	**	Pyrene + ?	202(100)101(53)57(39)88(32)71(27)200(22)203(16)201(16)		
32	2050	**	?	72(100)74(83)55(61)56(60)85(60)100(33)41(5)145(4)		
33	2088	**	Alkyl-alcohol or Alkane	57(100)70(66)83(70)97(53)111(23)125(8)208(3)		
34	2099	**	Heneicosane	71(100)85(74)57(70)99(21)113(9)127(4)218(2)		
35	2125	**	?	58(100)186(47)43(65)44(61)71(13)86(10)185(7)	Undecane,2-methyl	638
36	2150	**	C ≥ 21 alkane + ?	60(100)73(96)55(82)57(77)83(50)129(36)97(30)185(8)284(1)		

TABLE A-163. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 60F

GC Peak No.	Retention Index	Amount µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	SI x 10³
1	835	*	Tetrachloroethene	131(100)129(99)166(86)164(68)94(85)96(54)168(39)	Ethene,tetrachloro	416
2	850	*	Chlorobenzene	112(100)114(36)77(96)	Benzene,chloro	451
3	861	*	Ethylbenzene	91(100)106(96)56(61)105(46)77(40)	Benzene,1,2-dimethyl	402
4	879	*	Xylene	91(100)106(59)51(32)77(27)65(18)	Benzene,1,2-dimethyl	489
5	883	*	2-Butoxyethanol	57(100)87(22)99(9)116(2)		
6	910	*	Dihydromethylfuranone	56(100)85(49)43(47)100(4)		
7	931	**	Dihydronaphthalene	126(100)77(96)105(89)106(84)		
8	936	**	Dihydronaphthalene	93(100)92(93)126(83)125(61)128(65)127(56)		
9	965	*	C_3-Alkylbenzene + ?	106(100)99(97)120(77)		
10	953	*	C_3-Alkylbenzene	105(100)120(68)91(26)77(31)51(20)	Benzene,1-ethyl-3-methyl	626
11	960	*	C_3-Alkylbenzene	105(100)120(36)77(25)79(22)91(20)51(14)65(12)63(8)	Benzene,1-ethyl-2-methyl	602
12	976	**	C_3-Alkylbenzene	120(100)107(100)106(98)105(96)77(77)91(54)89(54)51(51)65(32)63(24)	Benzene,1-ethyl-2,4-dimethyl	360
13	982	*	Chloromethylbenzene	91(100)45(67)126(16)99(8)128(6)	Benzene,1-chloro-3-methyl	388
14	1092	**	Dichloromethylbenzene + ?	89(100)126(98)63(98)57(84)160(90)162(56)164(8)	Benzene,1-chloro-3-chloromethyl	363
15	1116	**	Dichloromethylbenzene + ?	107(100)106(99)136(99)125(81)127(22)160(18)162(12)		
16	1146	**	1,2,4-Trichlorobenzene + ?	182(100)180(100)184(68)74(97)85(88)109(77)145(72)147(44)	Benzene,1,2,3-trichloro	349
17	1178	*	Trichlorobenzene	180(100)182(92)184(28)74(72)109(58)145(55)	Benzene,1,2,3-trichloro	412
18	1276	*	Methylbenzothiazole	149(100)108(52)69(40)	Benzothiazole,2-methyl	619
19	1297	*	Trichloromethylbenzene	159(100)61(67)161(63)123(46)194(24)196(22)163(10)	Benzene,2,4-dichloro-1-chloro methyl	341
20	1339	*	Tetrachlorobenzene	216(100)214(80)74(80)108(79)218(48)220(10)	Benzene,1,2,4,5-tetrachloro	412
21	1365	*	Diphenyl ether	170(100)77(90)51(85)141(75)171(12)	Benzene,1,1'-oxybis	480
22	1911	**	Sebacate plasticizer	163(100)135(98)108(58)69(40)162(43)220(34)95(33)175(16)189(11)		
23	2514	**	Silicone	162(100)163(34)164(15)		
24	2725	**	Silicone	108(100)300(57)242(44)122(47)166(23)		

TABLE A-164. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 60E

GC Peak No	Retention Index	Amount, μg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10^3
1	860	*	C ≥ 6 Fatty Acid	74(100)87(37)85(36)57(36)59(28)41(22)43(20)	Butanoic Acid, 3-Methyl-, Methyl Ester	526
2	899	**	Methoxybenzene	108(100)65(70)78(66)51(16)63(15)93(17)109(8)	Benzene, Methoxy-	517
3	912	**	C ≥ 6 Fatty Acid	74(100)87(41)63(42)59(30)99(22)101(10)100(2)	Pentanoic Acid, 3-Methyl-, Methyl Ester	420
4	975	**	Chlorophenol	128(100)130(74)65(80)64(58)66(34)92(38)100(18)73(17)	Phenol, 2-Chloro-	477
5	1013	***	Phenol	94(100)66(83)65(60)55(11)50(10)95(11)	Phenol	468
6	1031	*	C ≥ 7 Fatty Acid	87(100)102(65)57(27)41(26)115(15)130(12)129(11)	Heptanoic Acid, 2-Ethyl-, Methyl Ester	342
7	1031	*	Chloromethylphenol + ?	107(100)108(48)77(68)79(32)51(20)142(30)144(10)		
8	1043	**	Methylphenol + #9	108(100)107(93)77(49)79(49)90(23)51(20)172(20)174(20)	Phenol, 2-Methyl-	316
9	1040	*	Benzoic Acid	105(100)77(96)51(36)136(30)	Benzoic Acid	566
10	1069	***	Chloromethoxybenzene	142(100)99(83)127(55)107(47)144(32)77(30)63(26)129(18)	Benzene, 1-Chloro-4-Methoxy-	395
11	1090	**	C ≥ 7 Fatty Acid + ?	74(100)87(52)55(26)59(21)127(14)129(6)	Hexanoic Acid, 5-Methyl-, Methyl Ester	333
12	1169	**	Dichlorophenol (methylated)	161(100)133(96)176(90)163(64)135(60)178(56)180(9)	Benzene, Dichloromethoxy-	555
13	1185	*	Thienopyridine C_7H_5NS	135(100)108(36)69(21)82(12)136(8)	Thieno[3,2-C] Pyridine	684
14	1190	*	C ≥ 8 Fatty Acid	74(100)87(55)143(10)		
15	1204	**	Chlorobenzoic Acid	139(100)111(41)75(27)50(12)113(14)141(32)170(27)172(9)	Benzoic Acid, 3-Chloro, Methyl Ester	739
16	1210	**	Dichlorophenol (methylated) + ?	128(100)130(32)65(42)100(22)141(7)143(6)176(11)178(7)		
17	1226	**	Dichlorophenol (methylated)	161(100)176(86)133(85)163(64)135(54)178(52)	Benzene, Dichloromethoxy-	560
18	1300	**	Trichlorophenol (methylated)	195(100)197(95)199(30)167(67)169(64)210(52)212(48)214(15)	Benzene, 1,2,4-Trichloro-5-Methoxy-	684
19	1333	**	Methoxy-1,2-Benzisothiazole	165(100)136(69)150(64)106(40)122(32)164(46)166(11)	1,2-Benzisothiazole, 3-Methoxy-	417
20	1371	*	Chlorophenoxyethanol	128(100)130(34)172(18)174(6)	Ethanol, 2-(4-Chlorophenoxy)-	516
21	1391	*	Dichlorobenzoic Acid	173(100)175(66)145(26)147(18)206(18)206(12)	Benzoic Acid, 3,4-Dichloro-	701
22	1419	*	Dimethylethyl-Benzodioxolone	177(100)149(28)91(18)178(12)192(11)	1,3-Benzodioxol-2-one, 5-(1,1-Dimethyl)-	289
23	1509	**	Dodecanoic Acid	74(100)87(74)55(29)143(14)183(5)185(3)214(2)	Dodecanoic Acid, Methyl Ester	436
24	1523	**	Methoxy-1,2-benzisothiazole	136(100)69(16)122(12)96(8)95(7)137(10)165(65)66(6)	1,2-Benzisothiazole, 3-Methoxy-	218
25	1551	**	Methylthiobenzothiazole	181(100)148(77)108(36)69(18)136(20)135(16)180(26)182(12)	Benzothiazole, 2-(Methylthio)-	712
26	1692	*	Subst.-Benzisothiazole	151(100)123(75)96(35)195(20) Weak Spectra		
27	1700	*	Tetradecanoic Acid	74(100)87(75)55(31)143(20)199(10)211(3)213(1)	Tetradecanoic Acid, Methyl Ester	382
28	1886	*	C ≥ 15 Fatty Acid + ?	74(56)87(38)	11-Octadecenoic Acid, Methyl Ester	369
29	1983	*	Subst.-Benzisothiazole	135(100)136(40)169(11)108*25)90(15)	Nonanoic Acid, Methyl Ester	584
30	2080	*	C ≥ 17 Fatty Acid	55(100)41(92)69(60)74(57)87(60)	11-Octadecenoic Acid, Methyl Ester	416

TABLE A-164. (Continued)

GC Peak No	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	EI x 10^3
31	2110	*	Octadecanoic Acid	74(100)87(76)43(65)55(34)143(24)199(10)	Heneicosanoic Acid, Methyl Ester	658

TABLE A-165. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 60E

GC Peak No	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	EI x 10^3
1	952	**	Methylpyridine	93(100)66(33)65(17)92(12)96(7)	Pyridine, 3-Methyl	515
2	1066	***	Methylaniline	106(100)107(72)77(17)79(13)89(7)51(7)	Benzenamine 4-Methyl	693
3	1085	**	? MW 126	41(100)40(90)126(80)43(77)67(52)68(49)86(28)125(10)127(6)	4(1H)-Pyrimidinone 2,6-Diamino	
4	1137	**	Dimethylaniline	121(100)120(67)106(95)77(22)91(16)103(10)		
5	1143	**	C_3-Alkylpyridine	121(100)120(92)106(92)77(21)91(16)	Pyridine, 3-Ethyl-5-Methyl	438
6	1169	*	C_3-Alkylpyridine	121(100)106(92)120(75)77(21)91(16)65(8)	Pyridine, 3-Ethyl-5-Methyl	359
7	1188	*	C_3-Alkylpyridine	106(100)121(91)120(52)77(20)91(15)103(12)65(10)	Pyridine, 3-Ethyl-4-Methyl	423

TABLE A-166. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 61VI

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.11		Air	44(100)
2	.13	< 1	Butene	41(100)39(50)56(40)
3	.15	1-10	Acetone	43(100)58(22)
4	.16	1-10	Diethylether	45(100)59(97)74(47)
5	.16	1-10	Dichloromethane	49(100)84(35)51(33)
6	.17	< 1	Carbon disulfide	76(100)44(12)78(8)
7	.25	< 1	Tetrahydrofuran	42(100)41(90)55(55)30(52)71(28)72(27)
8	.26	< 1	1,1,1-Trichloroethane	97(100)61(66)99(67)119(18)117(17)
9	.28	< 1	Benzene	78(100)
10	.34	< 1	Dichloropropane	63(100)62(70)41(52)39(40)65(32)76(25)
11	.36	< 1	Trichloroethylene	95(100)132,99(67)130(62)60(53)
12	.55	1-10	Toluene	91(100)92(60)
13	1.00	-(8)	I.S.	75(100)77(33)

TABLE A-167. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 61VE

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.12	---	Air	44(100)
2	.15	1-10	Acetone	43(100)58(28)
3	.16	~10	Diethyl ether	45(100)59(90)74(40)
4	.16	1-10	Dichloromethane	49(100)84(50)
5	.22	<1	Chloroform + I.S.	83(100)49(95)85(68)130(28)128(25)47(28)
6	.24	1-10	Tetrahydrofuran	42(100)41(55)71(27)72(26)
7	.26	<1	1,1,1-Trichloroethane	97(100)99(66)117(12)119(13)
8	.28	<1	Benzene	Benzene
9	.30	1-10	Cyclohexane	56(100)41(65)84(60)69(27)
10	.34	<1	Dichloropropane	63(100)62(71)41(50)39(37)65(31)76(25)
11	.61	<1	Dibromomethane	107(100)109(92)
12	.80	<1	Chlorobenzene	112(100)77(97)114(30)
13	1.00	~(8)	I.S.	75(100)77(33)
14	1.09	<1	Unknown hydrocarbon	109(100)95(90)67(43)81(40)123(12)
15	1.12	<1	$C_{10}H_{?}O$	55(100)69(88)83(82)41(78)125(30)
16	1.15	1-10	Unknown hydrocarbon	109(100)81(94)67(40)41(38)95(22)123(18)
17	1.18	1-10	Unknown hydrocarbon	81(100)109(38)41(35)55(32)67(27)138(6)

TABLE A-168. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 62VI

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.12	--	Air	44(100)
2	.15	1-10	Acetone	43(100)58(32)
3	.16	<1	Dichloroethylene	61(100)96(50)98(30)
4	.16	1-10	Dichloromethane	49(100)84(67)
5	.16	~1	Carbon disulfide	76(100)44(18)78(8)
6	.22	1-10	Chloroform	83(100)85(67)
7	.24	<1	Tetrahydrofuran + Chlorobutene	55(100)41(81)39(55)42(45)56(25)71(18)72(17)90(15)92(5)
8	.26	<1	1,1,1-Trichloroethane	97(100)99(67)61(62)119(12)117(10)
9	.28	~1	Benezene	78(100)
10	.33	<1	Dichloropropane	63(100)62(72)41(45)39(38)65(32)76(25)
11	.35	<1	Trichloroethylene	95(100)132(67)97(63)130(60)
12	.54	1-10	Toluene	91(100)92(55)
13	.67	<1	1,1,2,2-Tetrachloroethene	129(100)131(95)166(92)164(80)
14	.79	<1	Chlorobenzene	112(100)77(90)50,51(38)114(33)
15	1.00	-(8)	I.S.	75(100)77(33)

TABLE A-169. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 62VE

GC Peak No	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.10	--	Air	44(100)
2	.11	20-40	Vinyl Fluoride (T)	46(100)45(99)
3	.12	40-60	Ethyl Chloride	64(100)49(82)66(70)
4	.14	60	Diethyl ether	45,59,74(100)(Sat'd)
5	.15	30-40	Dichloromethane (?)	49(100) no 84,86
6	.16	∼1	Chloropropane (T)	42(100)41(27)59(8)63(5)78(2)
7	.19	∼10	Methoxy trimethyl silane	89(100)59(90)
8	.20	1-10	Unknown	45(100)43(80)41(30)57(20)87(15)133(2)
9	.22	100-1000	Unknown oxygen-containing compound	75(100)45(600)43(55)47(40)59(16)76(15)87(12)
10	.25	1-10	Dichloroethane	62(100)49(42)64(32)98(8)
11	.26	80-100	1,1,1-Trichloroethane	97(100)99(60)61(60)63(20)119(10)
12	.40	--	Silicone	147(100)73(25)
13	.51	∼10	2-Ethyl_1,3_Dioxolane (T)	73(100)45(50)57(12)101(3)
14	.55	∼1	Toluene	91(100)92(55)
15	.69	1-10	1,1,2,2-Tetrachloroethane	166,129(100)131(95)164(80)
16	1.00	-(8)	I.S.	75(100)77(33)

TABLE A-170. IDENTIFICATION OF COMPONENTS IN ACIDIC FRACTION OF SAMPLE NO. 62E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	RI x 10³
1	832	*	C ≤ 6 Fatty acid	45(100)87(72)43(67)59(36)88(14)99(7)		
2	836	*	C ≤ 6 Fatty acid	74(100)43(52)87(34)59(27)99(17)101(8)	Pentanoic acid, 3-Methyl Methyl Ester	510
3	840	**	Carbitol	45(100)59(34)72(24)104(3)103(2)	Ethane,1,1'-Oxy Bis(2-Ethoxy)-	630
4	885	*	C ≤ 6 Fatty acid	87(100)102(66)57(42)115(12)130(9)129(8)	Heptanoic acid,2-Ethyl, Methyl Ester	450
5	913	*	Methylphenol	108(100)107(89)79(49)77(48)51(22)90(24)109(8)	Phenol,2-Methyl-	586
6	1046	**	?	57(100)59(40)75(24)117(21)85(18)131(5)		
7	1278	**	Ethane,1,1'Oxybis(2-Ethoxy)	45(100)59(96)73(60)72(36)117(40)147(1)		
8	1372	*	Polypropylene glycol methyl ether	59(100)41(80)117(62)45(56)73(40)186(4)		
9	1418	*	Ethanol,2-[2-(2-Ethoxyethoxy)Ethoxy]	59(100)45(94)117(70)73(48)147(2)148(1)161(1)		
10	1435	*	N-4-Dimethyl benzenesulfonamide	91(100)65(32)155(16)121(12)185(14)186(1)	Benzenesulfonamide,N-4-Dimethyl	665
11	1722	**	Polypropylene glycol methyl ether	59(100)117(86)41(72)73(40)131(2)147(1)		
12	1884	*	C ≥ 15 Fatty acid	55(100)74(60)87(41)236(2)237(1)	10-Undecenoic Acid	583
13	1983	**	Polyproprylene glycol methyl ether	59(100)45(81)117(88)73(32)87(27)103(12)131(4)		
14	2109	*	Polypropylene glycol methyl ether	59(100)41(44)45(63)103(27)73(23)87(22)		
15	2150	*	Polypropylene glycol methyl ether	45(100)41(43)89(40)87(25)133(10)73(25)		
16	2249	**	Polypropylene glycol methyl ether	59(100)45(64)41(58)117(98)129(4)133(4)131(3)161(3)		
17	2513	**	Polypropylene glycol methyl ether	117(100)59(83)45(43)73(32)129(6)133(6)16(5)175(1)		
18	2765	**	Polypropylene glycol methyl ether	117(100)59(87)45(60)73(36)133(7)129(6)161(4)175(0.7)		

TABLE A-171. IDENTIFICATION OF COMPONENTS IN BASIC FRACTION OF SAMPLE NO. 62E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	RI x 10³
1	845	**	? MW 149	149(100)133(89)150(15)134(12)75(11)115(7)67(4)		
2	933	**	Silicone? MW 205	59(100)43(74)85(18)103(11)205(16)206(3)		
3	955	***	N-Butyl-1-butamine	44(100)86(96)41(21)57(18)129(13)	1-Butanamine, N-Butyl-	689
4	960	*	N-Butyl, N-Methyl-1-Butamine	58(100)100(76)44(49)86(24)143(9)129(3)	1-Butanamine, N-Butyl-N-Methyl	582
5	997	*	Silicone? MW 223	207(100)208(21)191(18)223(14)133(15)75(8)		
6	1087	**	?	59(100)41(55)45(49)73(33)103(25)		
7	1352	**	?	97(100)139(80)162(32)83(40)100(32)62(26)182(3)		

TABLE A-172. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 63VI

GC Peak No.	Relative Retention Time	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.12	--	Air	44(100)
2	.16	1-10	Acetone	43(100)58(30)
3	.16	1-10	C_2H_6S, e.g. Dimethyl sulfide	62(100)47(93)45(55)46(40)61(37)
4	.17	~10	Dichloromethane	49(100)84(35)
5	.22	1-10	Chloroform	83(100)85(67)
6	.25	<1	Tetrahydrofuran + 2 Chloro-2-butene	42(100)41(96)55(75)39(55)72(32)71(30)90(15)92(5)
7	.27	<1	1,1,1-Trichloroethane	97(100)99(67)61(50)119(15)117(14)
8	.29	<1	Benzene	78(100)
9	.34	<1	Dichloropropane	63(100)62(68)41(52)39(40)76(18)
10	.37	<1	Trichloroethylene	95(100)97,132(65)130(57)
11	.41	<1	Methylmethacrylate (T)	41(100)69(60)39(40)99(15)100(14)
12	.80	<1	Chlorobenzene	112(100)77(80)114(33)
13	1.00	-(8)	I.S.	75(100)77(33)
14	1.17	<1	Unknown	55(100)91(60)93(20)

TABLE A-173. IDENTIFICATION OF COMPONENTS IN VOLATILE FRACTION OF SAMPLE NO. 63VE

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum
1	.06	--	Air	44(100)
2	.10	1-10	Acetone	43(100)44(40)58(25)
3	.11	>1000	Dimethyl sulfide	45,46,47,61,62(100)
4	.45	1-10	Dimethyl disulfide	94(100)45(93)79(62)46(50)
5	1.00	(8)	I.S.	75(100)77(33)

TABLE A-174. IDENTIFICATION OF COMPONENTS IN NEUTRAL FRACTION OF SAMPLE NO. 63E

GC Peak No.	Retention Index	Amount, µg/l	Tentative Identification	Characteristic Ions in Mass Spectrum	Most Reasonable Biemann Match	
					Compound	S.I. x 10^3
1	1005	*	Chlorobenzene	112(100)77(82)51(30)114(32)50(27)	Benzene, chloro	452
2	1509	*	Methyl,4-chlorophenyl sulfone	139(100)111(92)75(54)141(32)113(30)190(4)192(1)		
3	1853	*	Benzene,1,1'-sulfonylbis	125(100)77(49)51(44)97(20)218(5)	Benzene,1,1'-sulfonylbis-	417
4	1917	*	Dibutyl phthalate	149(100)41(12)150(8)205(1)223(1)	1,2-Benzenedicarboxylic acid,butyl-2-methyl propyl ester	620
5	2174	***	Benzene,1,1'-sulfonylbis[4-chloro]-	159(100)75(74)111(52)161(36)286(8)288(5)290(1)	Benzene,1,1'-sulfonylbis[4-chloro-	338
6	2138	***	Benzene,1,1'-sulfonylbis[4-chloro]	75(100)159(99)111(90)50(64)161(65)286(16)288(11)290(2)	"	335